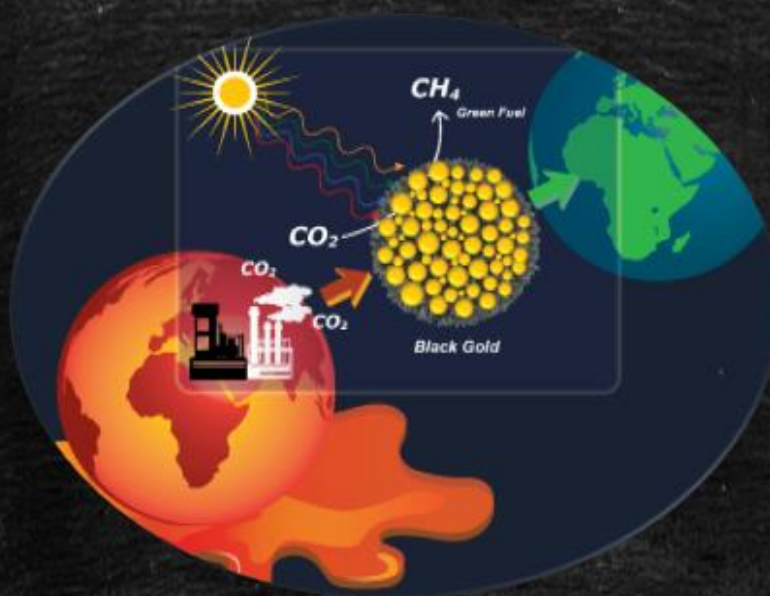




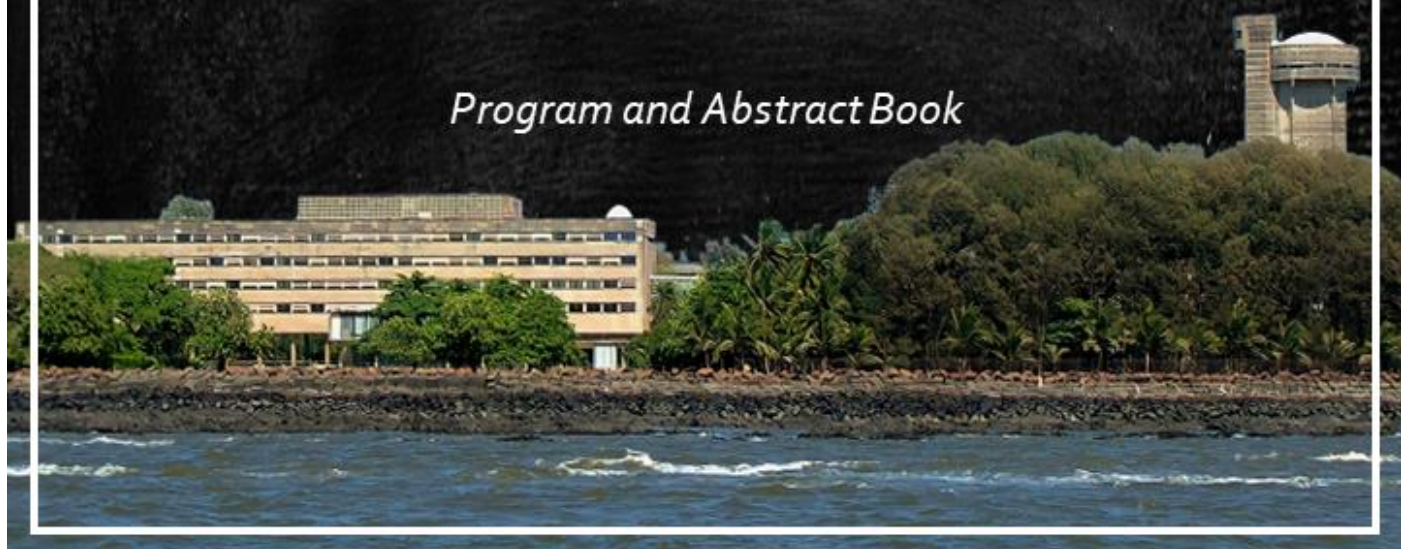
Conference on Advances in Chemistry for Energy and Environment (CACEE)

Homi Bhabha Auditorium, Tata Institute of Fundamental Research, Mumbai

16th Dec. to 20th Dec. 2024



Program and Abstract Book



Dr. Homi Bhabha
(Founder, TIFR, Mumbai)

"It is the duty of people like us to stay in our own country and build up outstanding schools of research such as some other countries are fortunate to possess." This was the vision that guided the Tata Institute of Fundamental Research which Homi Bhabha founded. The Institute was founded on 1st June 1945 with support from the Sir Dorabji Tata Trust." - Bhabha

"The pursuit of science and its practical application are no longer subsidiary social activities today. Science forms the basis of our whole social structure without which life as we know it would be inconceivable. As Marx said, "Man's power over nature lies at the root of history"...Science has at last opened up the possibility of freedom for all from long hours of manual drudgery and today we stand at the beginning of an age in which every person will have the fullest opportunity to develop himself spiritually to his fullest stature."
- Speech at the inauguration of TIFR on 1st June 1945.



"The key to national prosperity, apart from the spirit of the people, lies in the modern age, in the effective combination of three factors, technology, raw materials and capital, of which the first is perhaps the most important, since the creation and adoption of new scientific techniques can, in fact, make up for a deficiency in natural resources, and reduce the demands on capital. But technology can only grow out of the study of science and its applications."

-Opening statement of the GOI's Scientific Policy Resolution, 1958, of which he was one of the principal architects.

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Convenor

Prof. Vivek Polshettiwar

Professor (H), TIFR, Mumbai

Founder & Coordinator, CO₂India Network

President, Nanocatalysis Society

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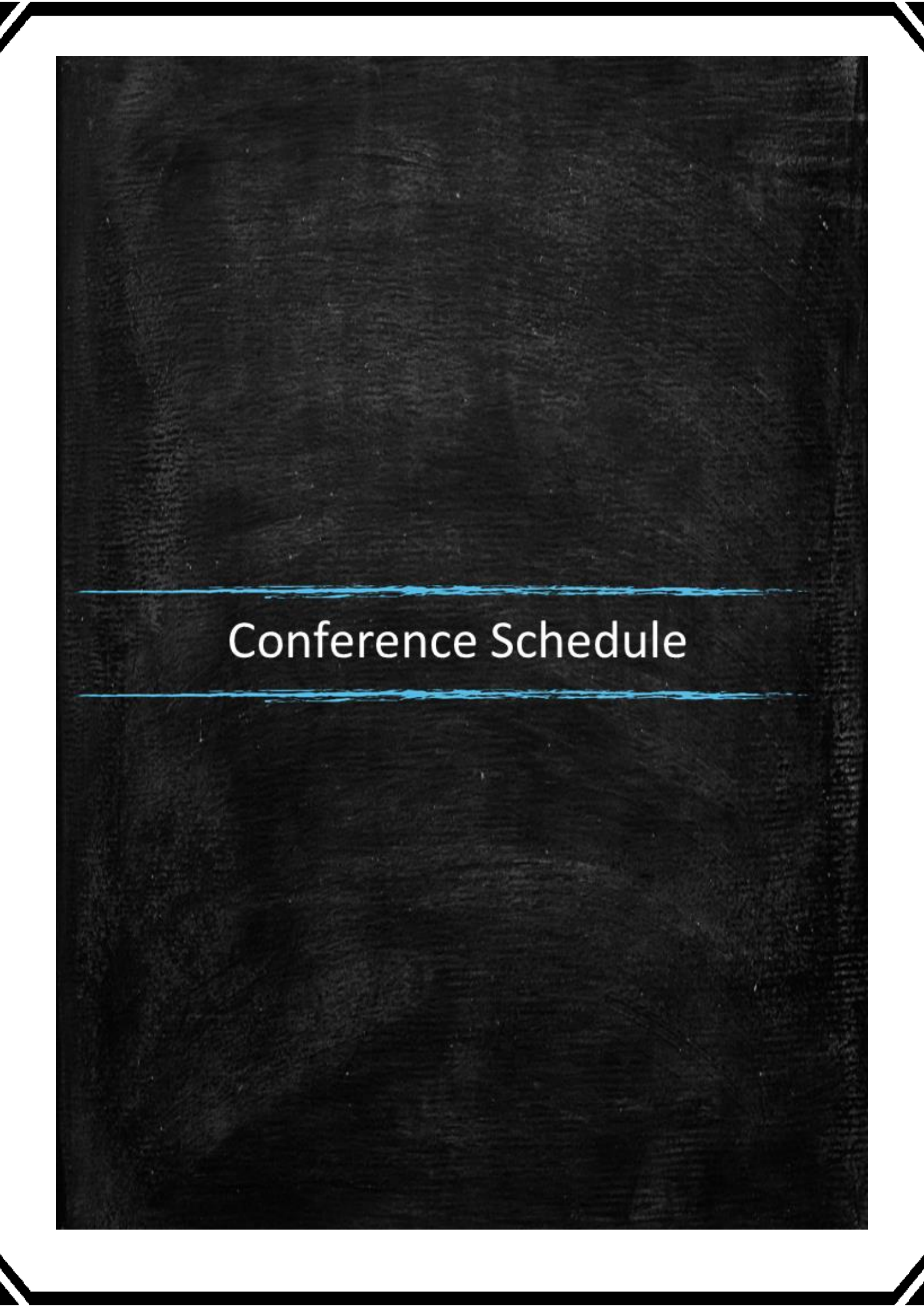
Preface

Addressing the urgent challenges of climate change, energy, and the environment requires the innovative use of chemistry. The proposed Conference on Advances in Chemistry for Energy and Environment (CACEE-2024) aims to bring together diverse branches of chemistry, materials science, spectroscopy, and computational studies to further advance this dynamic field of research. Our conference aims to foster discussions and innovative solutions by exploring the current fundamental understanding of chemistry to address energy and environmental challenges. Additionally, we will focus on enhancing light-matter interactions, designing and synthesizing novel materials, and employing in-situ techniques to study chemical processes.

The inaugural CACEE-2018 conference was held at TIFR, Mumbai, from January 10-12, 2018, attracting 250 participants and 45 distinguished speakers from around the world. CACEE-2020 was hosted virtually by TIFR, Hyderabad, due to the Covid pandemic. The third conference, CACEE-2022, took place from October 31 to November 4, 2022 at TIFR, Mumbai, in collaboration with the "CO₂India Network 1st Annual Meet," gathering 300 researchers and featuring 54 speakers across 19 sessions.

Looking forward to CACEE-2024 during 16-20 December 2024 at TIFR, Mumbai, our goal is to bring together researchers from various domains of chemistry. We aim to gather experts in novel material design, synthesis, and advancing mechanistic understanding through theory and spectroscopy. This conference will facilitate fundamental and technological advancements, and serve as a platform for exchanging ideas and fostering collaborations. The conference program will feature plenary, keynote, and invited talks by renowned researchers from around the world, along with oral and poster presentations by students and postdoctoral researchers.

Prof. Vivek Polshettiwar
Convenor, CACEE-2024
TIFR, Mumbai



Conference Schedule

CACEE-2024 SCHEDULE

Plenary (PL) - 40 min + 5 min Q&A; Keynote (KN) - 25 min + 5 min Q&A; Invited (IL) - 20 min + 5 min Q&A; Special Invited (SIL) - 15 min + 5 min Q&A

DAY-1: Monday 16th December 2024

7.00 - 8.30	Registration		
7.30 - 8.45	Breakfast		
9.00 - 9.30	INAGURATION		
Session 1- Auditorium (Chair- Prof. Sanjay Wategaonkar, Ex-TIFR, Mumbai)			
9.30 - 10.10	PL-1	Dr. Ashish Lele (CSIR-NCL, Pune, India) “Role of clean hydrogen in India’s energy transition - Opportunities and challenges”	
10.15 - 10.55	PL-2	Prof. Ramakrishna Sonde (IIT, Delhi, India) “CCUS the final bastion to net zero: Molecular insight to industrial impact”	
11.00 - 11.05	GROUP PHOTO (in Auditorium)		
11.05 - 11.30	TEA BREAK		
Session 2- Auditorium (Chair- Prof. D. Bhattacharyya, BARC)		Session 3- AG-66 (Chair- Prof. J. Varghese, IITM)	
11.30 - 11.55	KN-1	Prof. Kuo-Wei Huang (KAUST, KSA) “Fueling the future”	KN-3 Prof. Jitendra K. Bera (IIT, Kanpur) “Asking ligands to lend a hand: Rational design of 3d metal-based catalysts”
12.00 - 12.25	KN-2	Dr. Pieter Glatzel (ESRF, France) “Element-selective operando characterization of functional materials”	KN-4 Prof. Swadhin K. Mandal (IISER, Kolkata) “Metal-free catalysis for CO ₂ functionalization”
12.30 - 12.50	IL-1	Prof. Pramod P. Pillai (IISER, Pune) “Ligand-directed ammonia synthesis using visible light and quantum dots”	IL-3 Prof. C. N. Tharamani (IIT, Ropar) “Efficient economical energy harvesting from plastic and electronic wastes using human bodily motions”
12.55 - 13.15	IL-2	Prof. Vamsee Voora (TIFR, Mumbai) “Intermolecular interactions and dielectric screening effects on core-level shifts, and X-ray emission spectroscopy”	IL-4 Prof. Biswarup Pathak (IIT, Indore) “Machine learning for CO ₂ reduction reactions”
13.20 - 13.35	SIL-1	Dr. Chandrani Nayak (BARC, Mumbai) “In situ/Operando X-ray absorption spectroscopy for energy applications”	SIL-2 Dr. Meghna A. Manae (ETH Zurich, Switzerland) “Temperature-dependent tunnelling mechanisms in intersystem crossing pathways of carbenes”
13.40 - 14.30	LUNCH		

Session 4- Auditorium (Chair- Prof. Prashant V. Kamat, University of Notre Dame)		
14.30 - 15.10	PL-3	Dr. Anil Kakodkar (Chancellor, Homi Bhabha National Institute) “Energy options for India in the net zero world”
15.15 - 17.15	PANEL Discussion-1: “Net Zero India: Nuclear, Solar, and CCU Solutions” Panelists: Prof. Anil Kakodkar (Nuclear Energy), Dr. Ashish Lele (Green Hydrogen), Prof. Ramkrishna Sonde (CCU), Prof. Prashant Kamat (Solar Energy), Dr. Neelima Alam (Government Funding and Policy) Moderators: Dr. Arun Kumar Nayak (Head, Nuclear Controls & Planning Wing, DAE) and Prof. Vivek Polshettiwar (TIFR, Mumbai)	
17.15 - 17.45	TEA BREAK	
Session 5- Auditorium (Chair- Prof. Matthias Driess, Technical University Berlin)		
17.45 - 18.25	PL-4	Prof. Sara E. Skrabalak (Indiana University Bloomington, USA) “A nanocrystal conversion pathway to high entropy alloy electrocatalysts”
18.30 - 19.10	PL-5	Prof. Thalappil Pradeep (IIT, Madras, India) “Can water microdroplets make soil? A path to sustainable nanotechnology”
19.15 - 21.30	DINNER at TIFR	
END of DAY-1		

DAY-2: Tuesday 17 th December 2024							
8.00 - 8.45		Breakfast					
Session 6- Auditorium (Chair- Prof. Gadi Rothenberg, University of Amsterdam)							
9.00 - 9.40		PL-6	Prof. Prashant V. Kamat (University of Notre Dame, Notre Dame, USA) “Efficacy of photocatalysis for solar fuel generation”				
9.45 - 10.25		PL-7	Prof. Hirendra N. Ghosh (NISER, Bhubaneswar, India) “Ultrafast plasmon dynamics in non-stoichiometric near infrared active semiconductor nanocrystals”				
10.30 - 11.10		PL-8	Prof. Javier Garcia Martinez (University of Alicante, Spain) “Catalyzing the green revolution: Unlocking previously inaccessible chemical processes”				
11.15 - 11.45		TEA BREAK					
Session 7- Auditorium (Chair- Dr. Pieter Glatzel, ESRF)			Session 8- AG-66 (Chair- Prof. Tej Choksi, Nanyang Tech. Uni.)		Session 9- AG-69 (Chair- Dr. Soujanya Yarasi, IICT)		
11.45 - 12.10		KN-5	Prof. Subi J. George (JNCASR, Bangalore) “Light-harvesting organic heterostructures”	KN-7	Prof. Kanishka Biswas (JNCASR, Bangalore) “Phonon-glass electron-crystal like high performance thermoelectrics”	KN-9	Prof. Deepa Khushalani (TIFR, Mumbai) “Decoding photo-accumulation of charge in ionic carbon nitride - applications for

						solar battery and dark photo-catalysis”
12.15 - 12.40	KN-6	Prof. Kana M. Sureshan (IISER, Thiruvananthapuram) “Thermal topochemical polymerization reactions: Challenges and opportunities”	KN-8	Prof. Abhishek Dey (IACS, Kolkata) “Selectivity in CO ₂ reduction”	KN-10	Prof. Jagadeesh Rajenahally (Leibniz Institute for Catalysis, Germany) “Catalysis for sustainable and circular chemistry”
12.45 - 13.05	IL-5	Prof. Abhijit Shrotri (Hokkaido University, Japan) “Mitigating the poisoning effect of formate during CO ₂ hydrogenation using cobalt containing dual-atom oxide catalysts”	IL-6	Prof. Sachin R. Rondiya (IISc, Bangalore) “Edge states in low-dimensional halide perovskites: Sites of efficient exciton dissociation”	IL-7	Prof. G. Roy (IIT, Tirupati) “Biomimetic studies on the detoxification of highly neurotoxin organomercurials”
13.10 - 13.25	SIL-3	Mr. Rishi Verma (TIFR, Mumbai) “Plasmon-enhanced solar powered ‘hot electron’ catalysis in black gold-nickel”	SIL-4	Dr. Sayantan Mahapatra (University of Illinois, USA) “Probing photophysical and photochemical processes in a nanoscale gap”	SIL-5	Dr. Vitthal B. Saptal (Politecnico di Milano, Italy) “Pincer-type palladium sites in an asymmetrical covalent organic framework as a single-atom catalyst for Miyaura borylation and self-cascade coupling”
13.30 - 14.30	LUNCH					
Session 10- Auditorium (Chair- Dr. Sukhendu Nath, BARC)			Session 11- AG-66 (Chair-Prof. Amit Kumar, Pohang University of Science & Techn.)		Session 12- AG-69 (Chair- Dr. Manish Mishra, NCL)	
14.30 - 14.55	KN-11	Prof. Rahul Banerjee (IISER, Kolkata) “Reticular chemistry: From covalent organic frameworks to porous crystalline nitrogen doped graphite”	KN-12	Prof. Rajnish Kumar (IIT, Madras) “Role of materials in scale-up of renewable energy and CCUS for netzero India by 2070. How do we make it sustainable?”	KN-13	Prof. Nitin T. Patil (IISER, Bhopal) “Ligand-enabled redox gold catalysis”

15.00 - 15.20	IL-8	Prof. Chandra S. Sharma (IIT, Hyderabad) “From Earth to Mars: Pioneering metal-carbon dioxide (metal-CO ₂) battery solutions for a greener tomorrow”	IL-10	Prof. Debayan Sarkar (IIT, Indore) “Can visible light do selective dearomative C-H activation”	IL-12	Prof. Ritesh Haldar (TIFR, Hyderabad) “Tailored molecular diffusion in nanoporous material for separation and catalysis”
15.25 - 15.45	IL-9	Prof. Srabanti Chaudhury (IISER, Pune) “Microscopic understanding of dynamic catalysis using a discrete-state stochastic approach”	IL-11	Prof. Basker Sundararaju (IIT, Kanpur) “Asymmetric C-H bond functionalizations under cobalt catalysis”	IL-13	Prof. Sanjay K. Singh (IIT, Indore) “Low-temperature catalytic hydrogen production reactions”
15.50 - 16.15	Group Photo with KURTA (in lawn)					
16.15 - 17.30	PANEL Discussion-2: From Lab to Market: Breaking Barriers in Translating Fundamental Science Panelists: Prof. Javier Garcia Martinez (<i>University of Alicante</i>), Prof. Kuo-Wei Huang (<i>KAUST</i>), Prof. Rajnish Kumar (<i>IIT, Madras</i>), Mr. Aman Tandon (<i>Technip Energies</i>), Dr. Chiranjeevi Thota (<i>BPCL</i>), Dr. Pratik S. Dash (<i>Tata Steel</i>) Moderators: Prof. Gadi Rothenberg (<i>University of Amsterdam, Netherlands</i>) & Prof. Vivek Polshettiwar (<i>TIFR, Mumbai</i>)					
17.30 - 19.00	POSTER Session-1: P001 - P100 (+ TEA BREAK)			CO ₂ India Best Thesis Posters (+ Online Posters for those who are abroad)		
19.00 - 21.30	DINNER at TIFR					
END of DAY-2						

DAY-3: Wednesday 18 th December 2024		
8.00 - 8.45	Breakfast	
Session 13- Auditorium (Chair- Prof. Carsten Sievers, Georgia Institute of Technology)		
9.00 - 9.40	PL-9	Prof. Matthias Driess (Technical University Berlin, Germany) “Molecular strategies to meet expectations of chemistry in a sustainable world”
9.45 - 10.25	PL-10	Prof. Kamal K. Pant (IIT, Roorkee, India) “Enigma of CO ₂ and biomass conversion pathways to sustainable fuels through green catalysis”

10.30 - 11.15	PANEL Discussion-3: Editors' Insights for Navigating the Publishing Landscape Panelists: Prof. Malla Reddy Chilla (RSC), Prof. Sara Skrabalak (ACS), Prof. Carsten Sievers (Elsevier), Dr. Shreya Sarkar (Cell Press), Dr. Rohit Bhatia (Thieme) Moderators: Dr. Aayushi Arora (RSC), Ms. Gunjan Sharma (TIFR, Mumbai)				
11.15 - 11.45	TEA BREAK				
Session 14- Auditorium (Chair- Prof. Sudarshan Vijay, IITB)			Session 15- AG-66 (Chair- Dr. Santosh Gupta, BARC)	Session 16- AG-69 (Chair- Prof. M. Dharmapura, Manipal)	
11.45 - 12.10	KN-14	Prof. Kazuhiro Takanabe <i>(University of Tokyo, Japan)</i> <i>"Determination and perturbation of electron potentials in solid catalysts: Bridging the gap among thermal-, electro-, and photo-catalysis"</i>	KN-16	Prof. Ch Subrahmanyam <i>(IIT, Hyderabad)</i> <i>"Novel adsorbents derived from bio-waste for water treatment"</i>	KN-18 Prof. Diwan S Rawat <i>(Vice Chancellor, Kumaun University)</i> <i>"Navigating the expected and unexpected twists and turns of lead optimization: The discovery of clinical candidate for the treatment of Parkinson disease"</i>
12.15 - 12.40	KN-15	Dr. Paolo Longo <i>(Thermo Fisher Scientific, USA)</i> <i>"Introducing the Iliad - the first fully integrated advanced analytical L-shaped (S)TEM"</i>	KN-17	Prof. Ayan Datta <i>(IACS, Kolkata)</i> <i>"Buckling and defects in two - dimensional atomically thin monolayers"</i>	IL-16 (12.15-12.35) Prof. Manoj B. Gawande <i>(ICT, Jalna)</i> <i>"The Rise of single atom catalysts: Synthesis and catalytic applications"</i>
12.45 - 13.05	IL-14	Prof. Tej S. Choksi <i>(Nanyang Technological University, Singapore)</i> <i>"A multiscale understanding of how oscillating bubbles orchestrate chemistry in sonochemical reactors"</i>	IL-15	Prof. Tokeer Ahmad <i>(Jamia Millia Islamia, New Delhi)</i> <i>"Chemistry of heterogeneous catalysis for sustainable green hydrogen energy"</i>	IL-17 (12.40-13.00) Prof. Sandip Murarka <i>(IIT, Jodhpur)</i> <i>"Harnessing light to propel C-H functionalization"</i>
13.10 - 13.25	SIL-6	Dr. Prasenjit Das <i>(Technische Universität Berlin, Germany)</i> <i>"Multicomponent covalent organic frameworks: Design to function"</i>	SIL-7	Dr. Mahak Dhiman <i>(IIP, Dehradun)</i> <i>"Harnessing electrochemical power to convert CO₂ into C₄ oxyhydrocarbon and polymer"</i>	IL-18 (13.05-13.25) Prof. Komal Tripathi <i>(IIT, Roorkee)</i> <i>"Unleashing the potential of novel CO₂ transformation technologies"</i>
13.30 - 14.30	LUNCH				

Session 17- Auditorium (Chair- Prof. Kazuhiro Takanabe, University of Tokyo)			Session 18- AG-66 (Chair- Dr. Rohini Gupta, BASF)	
14.30 - 14.55	KN-19	Prof. C Malla Reddy (IIT, Hyderabad) “Dynamic molecular crystals”	KN-21	Dr. Chiranjeevi Thota (BPCL, Noida) “Green initiatives for sustainable future”
15.00 - 15.25	KN-20	Prof. Tapas K Maji (JNCASR, Bangalore) “Post-modified metal-organic frameworks for solar fuel production”	KN-22	Dr. Pratik S. Dash (Tata Steel, Jamshedpur) “Importance of CCUS in Indian steel industries: Roadmap for carbon neutrality”
15.30 - 15.50	IL-19	Prof. Prashant Kumar (Nanyang Technological University, Singapore) “Hybrid metamaterials with controllable twist”	IL-22	Dr. Sharan Shetty (Shell Technology Centre, India) “Computational insights in CO ₂ capture and conversion: An industrial perspective”
15.55 - 16.15	IL-20	Prof. Shinya Masuda (University of Tokyo, Japan) “Synthesizing robust Au cluster catalysts with defined numbers of Au atoms on heterogeneous supports using non-covalent ligand-support interactions”	IL-23	Prof. Prakash D. Vaidya (ICT, Mumbai) “Role of sorption-enhanced reactions in a circular carbon industry”
16.20 - 16.40	IL-21	Prof. Ananth G. Rajan (IISc, Bengaluru) “Machine learning-assisted exploration of materials and mechanisms for CO ₂ capture and conversion”	IL-24	Prof. Kaushik Ghosh (Institute of Nano Science & Technology, Mohali) “Multifunctional 2D material-based sensors and energy harvesting systems”
16.45 - 19.00	POSTER Session-2: P101 - P200 (+ TEA BREAK)			
19.00 - 21.30	DINNER at TIFR			
END of DAY-3				

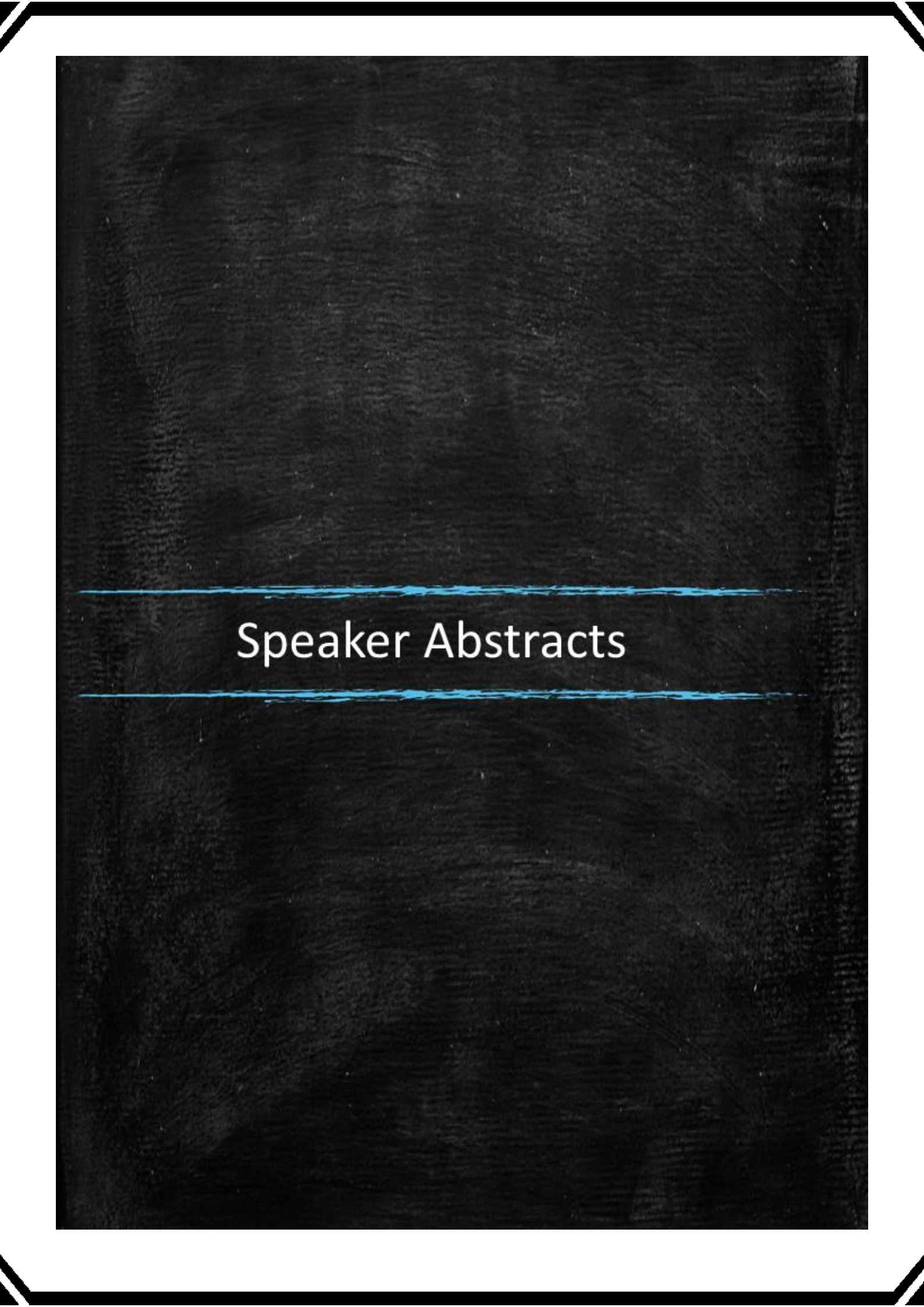
DAY-4: Thrusday 19 th December 2024		
8.00 - 8.45	Breakfast	
Session 19- Auditorium (Chair- Prof. Javier Garcia Martinez, University of Alicante)		
9.00 - 9.40	PL-11	Prof. Carsten Sievers (Georgia Institute of Technology, USA) “Creating reaction environments for mechanocatalytic upcycling of waste plastics”
9.45 - 10.25	PL-12	Prof. M. Lakshmi Kantam (Institute of Chemical Technology, Mumbai) “Design and development of heterogeneous catalysts for sustainable chemical industry”
10.30 - 11.10	PL-13	Prof. Gadi Rothenberg (University of Amsterdam, Netherlands) “What to do with CO ₂ ?”

11.15 - 11.45	TEA BREAK			
Session 20- Auditorium (Chair- Dr. Kaustava Bhattacharyya, BARC)			Session 21- AG-66 (Chair- Prof. Amartya Bose, TIFR)	
11.45 - 12.10	KN-23	Prof. Debabrata Maiti (IIT, Bombay) <i>"Utilization of CO₂ in synergistic triple catalysis for anti-Markovnikov hydrocarboxylation of industrial alkenes"</i>	KN-24	Prof. Jyotishman Dasgupta (TIFR, Mumbai) <i>"Photoredox organic transformations in water using host-guest charge transfer chemistry"</i>
12.15 - 12.35	IL-25	Prof. Abinaya Sampath (IIT, Gandhinagar) <i>"Hydrogen production from formic acid decomposition over supported Pd alloy catalysts: Role of oxygen in aqueous phase reactions"</i>	IL-28	Prof. R. S. Swathi (IISER, Thiruvananthapuram) <i>"On assessing the carbon capture performance of graphynes with swarm intelligence"</i>
12.40 - 13.00	IL-26	Prof. Amit Kumar (Pohang University of Science and Technology, South Korea) <i>"Catalytic nano-devices for sustainable chemical synthesis"</i>	IL-29	Prof. Koustuv Ray (IIT, Kharagpur) <i>"Catalytic processes using CO₂ for the chemical value chain: Catalyst formulation by developing structure-activity relationships"</i>
13.05 - 13.25	IL-27	Prof. Aditi Halder (IIT, Mandi) <i>"Enhancing the performance of rechargeable flexible batteries"</i>	IL-30	Prof. Shivnath Mazumder (IIT, Jammu) <i>"AI-driven discovery of asymmetric Pauson-Khand reactions: A new toolbox in a synthetic chemist's treasure"</i>
13.30 - 14.30	LUNCH			
Session 22- Auditorium (Chair- Prof. Ravindra Venkatramani, TIFR)			Session 23- AG-66 (Chair- Prof. Pradip Sarwade, MU)	
14.30 - 14.55	KN-25	Prof. Vivek Polshettiwar and Ms. Charvi Singhvi (TIFR, Mumbai) <i>"Trimetallic synergy and defects"</i>	KN-26	Prof. Vikram Vishal (IIT, Bombay) <i>"Role of CCS in India's efforts in decarbonization"</i>
15.00 - 15.20	IL-31	Prof. Joyanta Choudhury (IISER, Bhopal) <i>"Toward a carbon-neutral energy economy via recycling CO₂"</i>	IL-35	Prof. Sudip Chakraborty (Harish-Chandra Research Institute, Allahabad) <i>"Computational advancement towards efficient catalytic materials: Connecting a few Dots"</i>
15.25 - 15.45	IL-32	Prof. Sounak Roy (BITS Pilani, Hyderabad) <i>"Valorization of CO₂"</i>	IL-36	Prof. Akshai Kumar A S (IIT, Guwahati) <i>"Role of radical and organometallic pathways in Pincer-metal catalysis for generation of hydrogen, fuel & specialty chemicals"</i>
15.50 - 16.10	IL-33	Prof. Ekambaram Balaraman (IISER, Tirupati)	IL-37	Prof. R. Nandini Devi (CSIR-NCL, Pune)

		“CO ₂ to value-added polycarbonate diol”		“Designing catalysts and reactors for enhancing scalability”
16.15 - 16.35	IL-34	Prof. V. Ramanathan (IIT, BHU) “Chemistry and materials from India’s past: Illustrations and contemporary challenges”	IL-38	Prof. Shelaka Gupta (IIT, Hyderabad) “Towards rational design of transition metal catalysts for the upgradation of biorenewables”
16.40 - 19.00	POSTER Session-3: P201 - P306 (+ TEA BREAK)			
19.00 - 20.00	CULTURAL PROGRAM in Auditorium			
20.00 - 22.00	GALA DINNER at AMOEBA GARDEN, TIFR			
END of DAY-4				

DAY-5: Friday 20 th December 2024				
8.00 - 8.45	Breakfast			
Session 24- Auditorium (Chair- Dr. Pravin Walke Patil, MU)			Session 25- AG-66 (Chair- Prof. Atul Wankhade, VNIT)	
9.00 - 9.25	KN-27	Dr. Pankaj Gautam (SABIC, Limburg, Netherlands) <i>"Plastic circularity: Grand challenges in chemical recycling and a new class of polyolefins molecularly designed for circularity"</i>	KN-28	Prof. Santosh J. Gharpure (IIT, Bombay) <i>"New avenues in radical based approaches to heterocycles"</i>
9.30 - 9.50	IL-39	Dr. Mrinal R. Pai (BARC, Mumbai) <i>"Green hydrogen generation: A step towards net zero emissions"</i>	IL-44	Prof. Malay Patra (TIFR, Mumbai) <i>"Catalytic manipulation of cellular redox processes for enhanced cancer chemotherapy"</i>
9.55 - 10.15	IL-40	Prof. Ojus Mohan (IIT, Bombay) <i>"Computational catalysis for sustainability: Fuels from CO₂ and methane"</i>	IL-45	Prof. Sonali Das (IIT, Bombay) <i>"Multi-functional core-shell catalysts for conversion of carbon dioxide"</i>
10.20 - 10.40	IL-41	Prof. Kalaivanan Nagarajan (TIFR, Mumbai) <i>"Perturbing a chemical equilibrium through vibrational strong coupling"</i>	IL-46	Prof. Uttam K. Ghorai (Ramakrishna Mission Vidyamandira, Belur Math) <i>"Electrochemical synthesis of N-based products (green ammonia, green urea & nitric acid) under ambient conditions: Fundamental and translational Components"</i>
10.45 - 11.05	IL-42	Prof. Venkata Krishnan (IIT, Mandi) <i>"Development of efficient heterogeneous catalysts for sustainable plastic upcycling, biomass valorization, CO₂"</i>	IL-47	Prof. Manjesh Kumar (IIT, Delhi) <i>"Tuning the physicochemical attributes of catalytically active materials for better"</i>

		conversion and transfer hydrogenation reactions”		understanding of structure-property-performance triad”
11.10 - 11.30	IL-43	Prof. Vidya Avasare (Ashoka University, Sonapat) “Machine learning-driven discovery of Pincer complexes for enhanced CO ₂ utilization”	OL-1	Best Poster Oral-1 (10 mins Talk + 5 mins Q&A)
			OL-2	Best Poster Oral-2
11.35 - 12.00	TEA BREAK			
Session 26- Auditorium (Chair- Prof. Venkata Krishnan, IIT, Mandi)			Session 27- AG-66 (Chair- Dr. Mrinal R. Pai, BARC)	
12.00 - 12.15	CI-1	CO ₂ India Best Thesis Talk-1 (20 mins Talk + 10 mins Q&A)	OL-5	Best Poster Oral-5
12.15 - 12.30			OL-6	Best Poster Oral-6
12.30 - 12.45	CI-2	CO ₂ India Best Thesis Talk-2	OL-7	Best Poster Oral-7
12.45 - 13.00			OL-8	Best Poster Oral-8
13.00 - 13.15	CI-3	CO ₂ India Best Thesis Talk-3	OL-9	Best Poster Oral-9
13.15 - 13.30			OL-10	Best Poster Oral-10
13.30 - 13.45	OL-3	Best Poster Oral-3 (10 mins Talk + 5 mins Q&A)	OL-11	Best Poster Oral-11
13.45 - 14.00	OL-4	Best Poster Oral-4	OL-12	Best Poster Oral-12
14.00 - 14.45	LUNCH			
14.45 - 15.30	CONCLUDING CEREMONY			
END of DAY-5 and CACEE-2024				



Speaker Abstracts

Plenary Speakers

PL-1: Role of Clean Hydrogen in India's Energy Transition – Opportunities and Challenges

Ashish Lele

CSIR-National Chemical Laboratory, Pune, India.

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Abstract

India became a signatory to the historic Paris agreement in 2021 by announcing five important commitments to climate action. Recognizing the role of clean hydrogen in India's energy transition, the Prime Minister also announced the creation of India's National Green Hydrogen Mission (NGHM) in the same year. The NGHM aims to accelerate the creation of end-to-end hydrogen ecosystem in the country, with particular emphasis on hydrogen production, manufacturing of plant and machinery to produce clean hydrogen and enable exports through bilateral arrangements. Additionally, the mission also focuses on stimulating the innovation ecosystem and creation of several enabling platforms and tools to help the adoption of clean hydrogen use cases. In this talk, I will summarise the efforts made by R&D organizations such as CSIR to develop technologies across the hydrogen value chain and take them closer to commercialization in partnership with industry partners through pilot projects and creation of hydrogen valleys.

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Ashish's current interests in research, innovation and technology are in the areas of clean energy systems with particular focus on hydrogen ecosystem, new sustainable manufacturing paradigms for materials and chemicals in relation to climate change and circular economy, and structure-processing-property-performance relations in polymers and advanced materials.

Ashish is presently Director of CSIR-National Chemical Laboratory. Prior to that he was Senior VP and Head-Advanced Materials and Alternative Energy Group at Reliance Industries Ltd, and Chief Scientist and Head-Polymer Science & Engineering Div, CSIR-National Chemical Laboratory. He has Bachelor's degree in Chemical Engineering from University of Bombay, Department of Chemical Technology (presently ICT), PhD in Chemical Engineering from University of Delaware, USA, and was a Research Associate at the University of Cambridge, UK. Ashish is Fellow Indian National Science Academy, Indian Academy of Sciences and Indian National Academy of Engineering. He is recipient of Shanti Swaroop Bhatnagar Award in Engineering Sciences and Infosys prize in Engineering and Computer Science.

PL-2: CCUS the Final Bastion to Net Zero: Molecular Insight to Industrial Impact

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Abstract

Two and half decades of working in this field has been a roller coaster ride at both extremes. From being convinced on CCUS as the final answer to decarbonise the fossil to being sceptical about CCUS has been a very interesting yo-yo within me. The question that still begs for answers are the integrity of capture and conversion (or sequestration) to eliminate CO₂ from the equation and the life cycle energy invested in this process and consequent CO₂ burden in CCUS. That the current point source emissions from mega industrial complexes need major change in their emission profile - to switch from the post-combustion technologies to pre-combustion ones for ease of capture - the question still unanswered is after capture what?

And that is where molecular insights are critical. The talk highlights the possible pathways. That conventional thermo catalytic processes have limited role to play is given and hence the pathways like photo-electro-chemical processes using new molecular structures will have to come to central stage to make CCUS a credible option. The processes will have to be designed to operate near ambient conditions and hence electrochemistry or photochemistry will have to play out at the industrial scale. The core-shell structure of material rendering will be the need of the hour and this is a new exciting science waiting to be unleashed.

The talk presents some new ideas for young scientists to think and work upon. The focus is to present a criteria using some dimension and dimensionless numbers for screening ideas at a very basic level for potential implementation at large scale.

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Dr. Sonde began his career at Bhabha Atomic Research Center (BARC), where he excelled, receiving the Dr. Homi Bhabha Gold Medal. Specializing in nuclear energy, he contributed to isotope separation and heavy water technologies, earning further accolades, including a Golden Jubilee award from the Prime Minister. After 23 years, he transitioned to National Thermal Power Corporation (NTPC), where he established the "Energy Technologies" division (now NETRA) to advance thermal power, carbon capture, and solar hybridization. Dr. Sonde is currently a Professor of Practice at IIT Delhi, with additional roles in IIT Jammu and CSIR-NEERI. His work focuses on clean energy technologies, such as coal-to-methanol, hydrogen fuel cells, sodium-sulfur batteries, and CCUS, collaborating with leading research institutions. He chairs NITI Aayog's task force on methanol production and serves on multiple national committees addressing energy, environment, and water. He was awarded the prestigious Materials Research Society of India - MRSI Medal 2019. In 2021, he was elected as a Fellow National Academy of Sciences, India (NASI).

PL-3: Energy options for India in the net zero world

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Abstract

It is now becoming increasingly clear that the long term energy security of India is bound to face a formidable challenge because of net zero constraint. The presentation would cover a possible way forward and research inputs that can alleviate the situation. The long-term energy security of India is poised to face significant challenges as the country strives to achieve net-zero carbon emissions. This ambitious goal demands a delicate balance between sustained economic growth and the transition to sustainable energy systems, all while addressing India's rising energy demands. The presentation will delve into the intricate interplay of these factors, focusing on innovative strategies and research-driven solutions that can help mitigate the constraints posed by the net-zero target.

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Prof. Anil Kakodkar is a distinguished Indian nuclear scientist and mechanical engineer, known for his significant contributions to India's nuclear energy program. He served as the Chairman of the Atomic Energy Commission of India and Secretary to the Government of India in the Department of Atomic Energy from 2000 to 2009. A key architect of India's self-reliant nuclear energy program, he played a pivotal role in the development of the indigenous pressurized heavy water reactor (PHWR) technology and the operationalization of India's three-stage nuclear power program. He also contributed to India's nuclear tests at Pokhran in 1974 and 1998. Prof. Kakodkar has been a strong advocate for the peaceful use of nuclear energy, emphasizing its potential to address India's energy security. He is the recipient of numerous awards, including the Padma Vibhushan, Padma Bhushan, and Padma Shri.

PL-4: A Nanocrystal Conversion Pathway to High Entropy Alloy Electrocatalysts

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Abstract

High entropy alloys consist of equal or near equal amounts of five or more elements, being stabilized by their high entropy of mixing. Historically, high entropy alloys have been studied as structural materials, but with the development of synthetic pathways to high entropy alloy nanoparticles, their interest as catalysts has been growing. The direct colloidal synthesis of high entropy alloy nanoparticles is challenging given the different conditions under which various precursors must be reduced or decomposed.¹ To address this challenge, a nanocrystal conversion pathway to high entropy alloy nanocrystals has been achieved in which core@shell nanocrystals are colloiddally synthesized first and then annealed at elevated temperatures to facilitate intermixing and the formation of the high entropy alloy phase.² Here, the design of the precursor core@shell nanocrystals will be discussed, establishing that this nanocrystal conversion pathway is a general strategy to high entropy alloy nanocrystals.³ The catalytic performance of these nanocrystals will also be discussed as a function of composition for the oxygen reduction reaction, showing strong dependence on metal identity and degree of intermixing.^{4,5}

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Dr. Sara Skrabalak received her B.A. degree in chemistry from Washington University in St. Louis in 2002 where she conducted research with Professor William E. Buhro. She then moved to the University of Illinois at Urbana-Champaign where she completed her Ph.D. degree in chemistry in fall of 2006 with the tutelage of Professor Kenneth S. Suslick. She then conducted postdoctoral research at the University of Washington – Seattle with Professors Younan Xia and Xingde Li, designing nanomaterials for biomedical applications. She began her independent career in the Chemistry Department at Indiana University – Bloomington in 2008, where she was named the James H. Rudy Professor in 2015 and Robert & Marjorie Mann Chair in 2024. She is a recipient of both NSF CAREER and DOE Early Career Awards. She is a 2012 Research Corporation Cottrell Scholar, a 2013 Sloan Research Fellow, a 2014 Camille Dreyfus Teacher-Scholar, and recipient of the 2014 ACS Award in Pure Chemistry and 2015 Baekeland Award. In 2017, she was named both a Fulbright Fellow and Guggenheim Fellow as well as the recipient of Research Corporation's Frontiers in Research Excellence & Discovery Award. In 2020 Professor Skrabalak was named a fellow of the American Association for the Advancement of Science and assumed the roles of Editor in Chief for both *Chemistry of Materials* and *ACS Materials Letters*. Her research group focuses on nanomaterial design and synthesis for applications in catalysis, solar energy use, secured electronics, chemical sensing, and more.

PL-5: Can Water Microdroplets Make Soil? A Path to Sustainable Nanotechnology

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Abstract

Soil is formed from rocks, textbooks say. It is a slow process; one cm thick soil takes 200-400 years to form depending on conditions. Nanoscale particles are most essential constituents of soil which help in plant growth. We showed that common mineral particles break down spontaneously to form nanoparticles within milliseconds when encapsulated in charged water microdroplets. In our experiments, micrometer-sized minerals such as quartz and ruby were transformed into nanoparticles ranging from 5 to 10 nanometers. Computer simulations helped us to understand the process. This rapid weathering process could significantly contribute to soil formation, considering the widespread presence of charged aerosols in the atmosphere. The process could also be used to make soil industrially, to enhance agricultural productivity. The active surfaces of materials formed in microdroplets could lead to catalysis of relevance contributing to the biological evolution of the planet.

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Thalappil Pradeep is one of the most prominent researchers of India in chemistry and materials. He is a fellow of all the four major science and engineering academies of India and six in the world. He is an Institute Professor at the Indian Institute of Technology Madras (IITM), Chennai, India. He is the Deepak Parekh Institute Chair Professor and is also a Professor of Chemistry. He studied at the University of Calicut, Indian Institute of Science (IISc), UC Berkeley, and Purdue. His research interests are in molecular and nanoscale materials. He is an author of over 550 scientific papers in journals and is an inventor of over 100 issued patents. He is involved in the development of affordable technologies for drinking water purification and some of them have been commercialized. His pesticide removal technology has reached about 10 million people. His arsenic removal technology, approved for national implementation, is delivering arsenic free water to about 1.3 million people every day. Along with his associates, he has incubated seven companies and three of them have production units. He is the recipient of several awards including the Shanti Swaroop Bhatnagar Prize, BM Birla Science Prize, National Award for Nanoscience and Nanotechnology, India Nanotech Innovation Award, JC Bose National Fellowship and National Water Award. He has won The World Academy of Sciences (TWAS) prize in Chemistry for the year 2018. Nation conferred the civilian award, Padma Shri on him in 2020. He is also a recipient of the Nikkei Asia Prize, Prince Sultan Bin Abdulaziz International Prize for Water, VinFuture Prize and ENI award. Recently, he has won the International Excellence Award of Karlsruhe Institute of Technology, Germany and the Fellowship of Schroff Foundation. He is a Fellow of all the science and engineering academies of India, TWAS, American Association for the Advancement of Science, African Academy of Sciences, US National Academy of Engineering and Academia Europaea. He is the author of the introductory textbook, *Nano: The Essentials* (McGraw-Hill) and is an author of the monograph, *Nanofluids* (Wiley-Interscience) and an advanced textbook, *A Textbook of Nanoscience and Nanotechnology* (McGraw-Hill). He is on the editorial boards of journals such as *ACS Nano*, *Chemistry of Materials*, *Analytical Chemistry*, *Chemical Communications*, *Nanoscale*, *JPC Letters*, etc., and was an associate editor of *ACS Sustainable Chemistry & Engineering* for ten years. He is now an Associate Editor of *ACS Sustainable Resource Management*. He has authored popular science books in English and Malayalam and is a recipient of Kerala Sahitya Akademi Award for knowledge literature. He has received the *Lifetime Achievement Research Award* of IITM and *Distinguished Alumnus Award* of IISc. As part of philanthropy, he supports a school in his village where 500 students are on rolls.

PL-6: Efficacy of Photocatalysis for Solar Fuel generation

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Abstract

Photocatalysis is considered to be an useful approach to generate solar fuels (e.g., H_2) using sunlight. Despite the 50+ years of research, photocatalysis lags behind electrocatalysis. For effective utilization of semiconductor nanocrystals in photocatalysis, the undesirable intrinsic charge recombination (at early time scale) and back electron transfer (longer timescale) need to be suppressed. The laser pulse irradiation and steady-state irradiation experiments map out timescales of forward and back electron transfer events that dictate the overall photocatalytic reduction process. However, the kinetic parameters and photoconversion efficiency measurements reported in the literature vary based on the type of photoirradiation and experimental conditions. Intense short-lived laser pulse excitation provides an opportunity to probe early events in excited semiconductor nanoparticle assembly, but they do not provide complete assessment of a photocatalytic process or echo the intricacy of realistic operative conditions. Effort to correlate ultrafast measurements to a photocatalytic performance should be accompanied by steady-state irradiation experiments. An important kinetic parameter overlooked in majority of photocatalytic studies is the back electron transfer process. The control of back electron transfer through proper surface modification or separation of reductive and oxidative processes can increase the net electron transfer efficiency or photocatalytic efficiency of a semiconductor system.

Designing a hybrid semiconductor nanocrystal:cocatalyst assembly in a polymer membrane is an effective approach to direct the flow of photogenerated charge carriers. The photocatalytic semiconductor/metal membrane when inserted between the two compartments of an H-cell, serves the dual purpose of generating hydrogen while separating the oxidation and reduction products. The talk will focus on preparing photocatalytic membrane and their effectiveness in solar fuel production and some of the key factors that dictate the efficiency of solar fuel generation.

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Prashant V. Kamat is a Rev. John A. Zahm, C.S.C., Professor of Science in the Department of Chemistry and Biochemistry and Radiation Laboratory at the University of Notre Dame. He is also a Concurrent Professor in the Department of Chemical and Biomolecular Engineering. Professor Kamat has for nearly four decades worked to build bridges between physical chemistry and material science to develop advanced nanomaterials that promise cleaner and more efficient light energy conversion. He has published more than 500 scientific papers that have been well recognized by the scientific community. Thomson-Reuters has featured him as one of the most cited researchers each year since 2014 (2014 -2023). He is a Fellow of ACS, ECS, MRS and AAAS. He is also Pravasi Fellow of the Indian National Science Academy. He is currently serving as the Editor-in-Chief of *ACS Energy Letters*.

PL-7: Ultrafast Plasmon Dynamics in Non-stoichiometric Near Infrared Active Semiconductor Nanocrystals

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Abstract

Surface plasmon resonance (SPR) in nanomaterials (NMs) facilitates the generation of hot carrier (electron-hole) through plasmon decay and has garnered substantial and increasing attention over the past two decades. Plasmonic NMs have numerous unique properties like high extinction co-efficient, long-range light absorption (Visible to IR), cost-effectiveness and easy to manipulate their physical properties. These attributes render them highly promising materials for multiple applications, including photocatalysis, photodetectors, nanophotonics and photothermal therapy etc. In the present talk we will discuss ultrafast plasmon dynamics in non-stoichiometric Cu_{2-x}Y ($\text{Y}=\text{S}, \text{Se}$) semiconductor nanocrystals (NCs). Transient spectra exhibit extended absorption span over entire infrared region, which is plasmon excitation or hot hole transition within the valence band of NC. Following transient kinetics we have monitored hole-hole, hole-phonon and phonon-phonon scattering, respectively. We have also demonstrated dynamics of hot hole delocalization and transfer dynamics in a p-n hetero-junction consisting of Cu_{2-x}Se and CdSe/CuInSe . Finally, we have successfully unraveled the process of plasmon-induced hot hole extraction, whereby hot holes are transferred from gold (Au) to Cu_{2-x}Se , within the framework of dual plasmonic hybrid nanocrystals (HNCs) comprising $\text{Au@Cu}_{2-x}\text{Se}$. These findings will open up a new avenue for harvesting visible to near infrared photon for the development of modern solar cells, photodetector and fast nanophotonic device application.

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Currently Director of National Institute of Science Education and Research, Bhubaneswar, Odisha. His current research interests include ultrafast interfacial charge carrier transfer and relaxation dynamics in semiconductor nanoparticles, hybrid nanostructures, perovskite, plasmonic and 2D materials using different ultrafast techniques which includes Femtosecond pump-probe broad-band (UV-Vis-NIR) and Terahertz spectrometer. Prof. Ghosh has published more than 240 research papers in highly reputed International Journals. His research accomplishments have been recognized through awards and fellowships such as INSA Young Scientist (1998), INSA A. K. Bose Memorial Award (2000), Homi Bhabha Science & Technology Award (2010), DAE-SRC Outstanding Investigator Award (2012), C. N. R. Rao National Prize for Chemical Research (2014), CRSI Bronze Medal (2011) CRSI Silver Medal (2022) and J C Bose National Fellowship from DST, Govt. of India. He is a fellow of all three major academia of India: Fellow of National Academy of Science (FNASc), Fellow of Academy of Science (FASc), and Fellow of Indian National Science Academy (FNA). He also became Fellow of National Academy of Engineering (FNAE), New Delhi, 2023.

PL-8: Catalyzing the Green Revolution: Unlocking Previously Inaccessible Chemical Processes

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Abstract

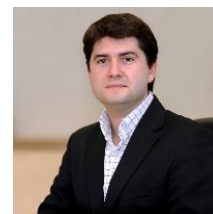
During the presentation, I will describe a new strategy for the synthesis of superior hierarchical catalysts, which lack long-range order but at local scale contain zeolite building units. [1,2] In fact, they are made out of fragments of one or even various zeolite structures and display improved accessibility, strong acidity, and excellent stability. Because of these features, they effectively catalyze reactions involving very bulky molecules, which currently are produced using highly corrosive homogenous catalysts (Fig. 1). To achieve this goal, we built on a well-known technique, namely the interconversion of zeolites, which we interrupted at different times to yield the desired amounts of building units of the zeolites involved. The addition of quaternary ammonium surfactants during their preparation allows the development of well-defined mesoporosity and large surface areas. Using this simple procedure, we were able to produce families of materials with controlled amounts of different zeolitic building units and, consequently, optimize their catalytic performance for various reactions including Friedel-Crafts alkylations and Claisen-Schmidt condensations, and the cracking of 1,3,5-triisopropylbenzene. An important advantage of this strategy is that the physicochemical properties and, therefore the catalytic performance, of the hierarchical catalysts can be finely tuned by simply stopping the interzeolite transformation at different times. This creates countless opportunities for the development of hierarchical catalysts [3] with optimized properties and superior catalytic performance for those reactions in which zeolites present significant diffusion limitations (Fig. 1). This paves the way for the fabrication of hybrid hierarchical catalysts with optimized properties for those processes in which the combined use of different zeolites yields improved performance.

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Professor of Inorganic Chemistry and Director of the Molecular Nanotechnology Lab, a world-leading research center dedicated to the synthesis and application of nanostructured materials for the sustainable production of chemicals and energy at the University of Alicante, Spain. Founder of Rive Technology, a technology-based company commercializing nanostructured catalysts that significantly reduce CO₂ emissions while increasing energy efficiency. In 2019, W. R. Grace acquired this technology and is now commercializing it globally. President of the International Union of Pure and Applied Chemistry (IUPAC) for the 2022-2023 biennium. He previously served as Vice President, member of the Executive Committee, and Vice President of the Division of Inorganic Chemistry. Javier is an Honorary Fellow of the Royal Society of Chemistry, and in 2018 he received the Kathryn C. Hach Award for Entrepreneurial Success from the American Chemical Society.

PL-9: Molecular Strategies to Meet Expectations of Chemistry in a Sustainable World

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Abstract

The expectations for chemistry to play a more decisive role than ever before in providing innovative solutions for a sustainable world are increasing. Challenges include the improvement of catalysts for efficient energy conversion, storage and selective transformation of chemicals on a relevant production scale with zero carbon emission in a scheme of economically feasible circular chemistry. We study the transformation of molecules-to-materials at low temperature which offers tremendous opportunities to produce unprecedented types of catalytic materials for long-term stable electrochemical applications. Using suitable molecular precursors for synthesizing functional inorganic nanomaterials and interfaces allows for reliable control over uniform particle size distribution and stoichiometry which is key to understand, improve and boost performance-relevant properties in electrocatalysis. [1-4] The approach enabled us to uncover composition-structural dynamic relationships using operando techniques. In my talk, I would like to discuss selected achievements and challenges of the molecular precursor approach in the light of recent developments of molecule-to-thin film materials synthesis for renewable energy applications, relevant for the oxygen evolution reaction (OER), hydrogen evolution reaction (HER) and biorefinery. Electrochemical water-splitting into hydrogen (H₂) and selective oxygenation of renewable chemicals from biorefinery is widely regarded as a promising approach to producing environmentally-friendly fuel for future energy supply.

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Matthias Driess studied Chemistry and Philosophy of Science at the Ruprecht-Karls University of Heidelberg (Germany) where he also received his PhD. He has been a postdoctoral fellow at the University of Wisconsin at Madison, U.S.A., before finishing his habilitation at the University of Heidelberg. From 1996 he was appointed as full-professor for Inorganic Chemistry at the Ruhr University Bochum, and since 2004 he holds a chair for organometallic chemistry and inorganic materials at the Department of Chemistry of the Technical University Berlin. He served as spokesperson of the Cluster of Excellence UniCat from 2007-2019, is director of the UniCat-BASF joint lab BasCat and scientific director of Chemical Invention Factory CIF, a pre-start up center for entrepreneurs from the molecular sciences. He is a member of the German National Academy of Sciences Leopoldina, the Berlin-Brandenburg Academy of Sciences and Humanities, the European Academy of Sciences and has published more than 460 scientific papers in peer-reviewed journals. His research is focusing on functional organometallic chemistry of earth abundant elements, energy material science and technology, electrocatalysts, artificial fuels, chemical energy storage and circular chemistry.

PL-10: Enigma of CO₂ and Biomass Conversion Pathways to Sustainable Fuels through Green Catalysis

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Abstract

The drive to decrease consumption of fossil fuels and expanding capacity for renewable energy, opens up the exploration of emerging routes to harness this energy for the sustainable materials, chemicals, and fuel production. Biomass represents a promising source as a precursor for these commodities due to its natural ability to sequester CO₂ in multi-carbon organic molecules. Thermochemical methods coupled with electrochemical approaches for upgrading biomass are hence intriguing, however there is an urgent need to clearly evaluate this emerging field and to unlock the opportunity space via recognizing best suited pathways. We contribute in this field by offering comprehensive and quantitative assessments of thermochemical conversion including gaseous (H₂, syngas, sustainable aviation fuel) and liquid products (bio-oil), solid products (bio-char), electrochemical reduction, oxidation of biomass-derived compounds including polyols, furans, carboxylic acids, amino acids, and lignin, with focus on developing the state-of-the-art facilities for complete value chain.

In parallel, despite the commercial success of syngas (3-5 vol.% of CO₂), a comprehensive understanding of catalyst formulations and reactor designs for converting pure CO₂ has yet to be realized. The talk will comprise of what has been achieved to date, exploring how the field has evolved, and advancements achieved. A particular focus will be given to different catalyst formulation/reactor design and critical assessment on the validity and novelty of various hypotheses. Also, attempts to develop an integrated approach including catalyst design to reactor kinetic to scaleup will be discussed.

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Prof. Vivek Polshettiwar research interests are within the domain of advanced nanomaterials and nanocatalysis for harvesting solar energy and the transformation of carbon dioxide into value-added chemicals and fuels. The work of his group in the nanocatalysis realms of "Black Gold" and "Defects" chemistry represents a quintessential example of how fundamental science can drive innovation in applied research. He is the recipient of the prestigious ORISE Research Fellowship at US-EPA. He also received an Asian Rising Star lectureship at 15th Asian Chemical Congress (ACC), Singapore (2013), from Nobel Laureate Professor Ei-ichi Negishi. In 2015, he was admitted as a Fellow of the Royal Society of Chemistry (RSC), United Kingdom. He was awarded a Bronze medal by the Chemical Research Society of India (CRSI), India. He was awarded the prestigious Materials Research Society of India - MRSI Medal 2019. In 2021, he was elected as a Fellow National Academy of Sciences, India (NASI). He received the 2022 IUPAC-CHEMRAWN VII prize for green chemistry from IUPAC. In 2023, he received the Falling Walls Award in Physical Sciences. In 2024, he was elected as a Fellow Indian Academy of Sciences. In 2024, he was Awarded Prestigious Vigyan Yuva-Shanti Swarup Bhatnagar (VY-SSB) Award by the President of India.

PL-11: Creating Reaction Environments for Mechanocatalytic Upcycling of Waste Plastics

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Abstract

Diversion of waste plastics from landfills and the environment is one of the big challenges of modern society. Some waste plastic streams can be reused or recycled, but chemical recycling will be critical to reintroduce the majority of plastics products into value chains. Mechanochemical processes offer a unique option for converting these solid feedstocks in excited environments created from mechanical collisions in a ball mill or similar device.

The depolymerization of poly(ethylene terephthalate) (PET) occurs readily when the polymer is milled with NaOH.¹ To understand the reaction at impact sites in detail, a 2.5 cm steel ball is dropped on a NaOH-coated PET film from a 1.07 m to have the same impact velocity as in a shaker mill at 30 Hz. Raman microscopy shows a gradient of PET depolymerization from 3% at the edge of the crater to 27% in the center.

When poly(styrene) is milled, styrene is produced at a constant rate and selectivity alongside minor products including oxygenates like benzaldehyde.² Continuous monomer removal during reactor operation is critical for avoiding repolymerization. A thermodynamic analysis shows that the cleavage of olefin monomers from chain end radicals is thermodynamically limited.³ Thus, it will be critical to generate more energetic and longer-lived reaction environments to increase the efficiency of this reaction.

An alternative approach to generate a driving force for depolymerization reactions is to couple the chain cleavage reactions with hydrogenation or oxidation of the fragments. For example, mechanocatalytic depolymerization of poly(ethylene) occurs when the polymer is milled hydrogen peroxide as an oxidant and an iron oxide catalyst. This leads to partial oxidation in random positions of the backbone followed by cleavage of C-C bonds.⁴

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Carsten Sievers obtained his Diplom and Dr. rer nat. degrees in Technical Chemistry at the Technical University of Munich, Germany. Under the guidance of Prof. Johannes A. Lercher, he worked on heterogeneous catalysts for various petrochemical processes. In 2007, he moved to the Georgia Institute of Technology to work with Profs. Christopher W. Jones and Pradeep K. Agrawal as a postdoctoral fellow. His primary focus was the development of catalytic processes for biomass depolymerization and synthesis of biofuels. He joined the faculty at the Georgia Institute of Technology in 2009. His research group is developing catalytic processes for the sustainable production of fuels and chemicals. Specific interests are catalyst deactivation and regeneration, mechanocatalysis, plastics upcycling, catalytic processes in water, surface chemistry of complex molecules, production of value-added chemicals from biomass, operando spectroscopy, and CO₂ capture and conversion. He published over 120 peer-reviewed papers. He is one of the Chairs of the 29th North American Meeting of the North American Catalysis Society (NAM29) and Deputy Editor-in-Chief of Applied Catalysis A: General.

PL-12: Design and Development of Heterogeneous Catalysts for Sustainable Chemical Industry

Prof. M. Lakshmi Kantam

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Abstract

Catalysis is a highly demanded technology for sustainable society and drives innovation in many other fields. Achieving the high catalytic selectivity is the goal of catalysis science in 21st century. Today over 90 % of all industrial chemicals are produced with the aid of catalysts. World catalyst demand is forecast to grow to \$34.1 billion in 2025 and earlier global sales of catalysts is around 20.6 billion dollars. The catalysis of organic reactions by homogeneous and heterogeneous catalysts remains a vibrant field of scientific inquiry. It attracts a diverse group of scientists with specialties spanning synthetic organic chemistry, inorganic chemistry, surface science, material science, reaction engineering and computational modeling.

Hydroxyapatite (HA) is a hydrated calcium phosphate material, which is an important biomaterial because of its similarity to the mineral component of mammalian bone. We have utilized these materials, and their metal exchanged materials as catalysts for C-C and C-N coupling reactions. Similarly, hydrotalcites and anionic clays have been exchanged with different metal ions and successfully applied in a number of organic transformations, for example: palladium exchanged catalysts in C-C coupling reactions. Reactive nanocrystalline metal oxides are newly discovered materials that could change dramatically the way these organic transformations are carried out. Nanostructured metal oxides are widely used in catalysis where the acidic/base properties and the catalytic activities are closely related to the size and morphology of the oxides. We have been exploiting different nanocrystalline metal oxides prepared by Prof. Klabunde for a number of organic reactions viz., Claisen-Schmidt, Wadsworth–Emmons, Wittig, aldol, asymmetric epoxidation, Henry, Michael, and hydrosilylation reactions etc. Over recent years, research has been going in the field to find alternatives to fossil fuels due to their depletion. Nowadays, most of the research is focused on synthesizing high-value-added chemicals from biomass as a renewable source for the alternative of fossil fuels. Our work on conversion of biomass to value added chemicals will be presented.

An overview of our work on the design and development of catalysts for green, and economical processes & technologies for chemical industry will be presented.

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Dr. Mannepalli Lakshmi Kantam is a distinguished Indian scientist and former Director of CSIR-IICT, Hyderabad. With a Ph.D. from Kurukshetra University (1982), she has made pioneering contributions to catalysis, focusing on sustainable and atom-economical processes. Her innovations include nanomaterial-supported catalysts, recyclable heterogeneous systems, and catalytic technologies for converting plastics into fuel. With over 260 publications, 43 US patents, and mentorship of 27 Ph.D. scholars, Dr. Kantam has received prestigious accolades, including the Lifetime Achievement Award from the Indian Chemical Society and a Fellowship of the National Academy of Sciences, India. She has also held leadership roles such as President of the Catalysis Society of India and adjunct professorship at RMIT University, Australia.

PL13: What to do with CO₂?

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Abstract

CO₂ emissions are a serious global problem. Hence the **Paris Agreement** and the **COP meetings**, where 118 countries agreed on reducing emissions and fighting climate change. Their main goals are keeping global warming below 2 °C, and reaching net-zero GHG emissions by 2050.¹ **Yet is this realistic?** GHG emissions may be everyone's long-term problem, but they are nobody's short-term problem. The benefits from the free energy stored in fossil fuels, combined with humans' fear of taking risks, create enormous barriers. In the 1st part of the lecture, I will show that **we cannot reach the goals of the Paris Agreement**. We must prepare to adapt to living in a world that is 3–4 °C warmer on average than pre-industrial times.² Meanwhile, since we are emitting so much CO₂, can we perhaps turn some of it into something useful? In the 2nd part of the lecture, I will give an overview on our group's recent work on **carbon capture and utilisation**, and examine ways for turning CO₂ emissions into useful products.^{3,4} We cannot solve the global CO₂ problem, but we can create small-scale alternatives that contribute to local sustainable development.

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Gadi Rothenberg is Professor and Chair of Heterogeneous Catalysis and Sustainable Chemistry at the University of Amsterdam. And Distinguished Visiting Professor at Tsinghua University. He teaches courses on catalysis and workshops on scientific writing, communication and innovation. Rothenberg has published four books and 245 peer-reviewed papers, invented 16 patents and founded four companies. His current research interests include clean energy, electrocatalysis, and creating value from waste. In 2023 he served as the Technical Director CO₂ and Circular Economy at the Shanghai Institute for CleanTech Innovation.

Keynote Speakers

KN-1: Fueling the Future

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Abstract

To reduce the environmental footprint of modern societies and address the limitations of fossil resources, the projected increase in global energy demand must go along with the implementation of low-carbon energy production and carrier systems. In this presentation, the current energy status and future options will be discussed and compared. It will then be concluded by introducing our research efforts in utilizing formic acid as a NET-ZERO hydrogen/energy carrier and e-fuel.

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Kuo-Wei Huang received his B.S. degree from National Taiwan University as a Yuan T. Lee Fellow and his Ph.D. degree from Stanford University as a Regina Casper Fellow. Before joining KAUST as a founding faculty member, he had been an Assistant Professor at the National University of Singapore and a Goldhaber Distinguished Fellow at Brookhaven National Laboratory. The research interests of his group include CO₂ utilization, hydrogen storage, small molecule activation (particularly on the PN³(P) ligand platform his group has developed and pioneered), and computational and kinetic mechanistic studies of catalysis. He is a co-author of over 320 peer-reviewed publications and a co-inventor of over 40 patents and applications. He has received numerous recognitions, including Appreciation of distinguished teaching contribution, Ministry of Education, KSA (2017), Rising Stars Lectureship, 41st International Conference on Coordination Chemistry (2014), SABIC Chair Professorship (2013-2016), Asian Rising Stars Lectureship, the 15th Asian Chemical Congress (2013). He was highlighted as “Pioneers and Influencers in Organometallic Chemistry” by *Organometallics* in 2020.

KN-2: Element-Selective *Operando* Characterization of Functional Materials

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Abstract

X-ray spectroscopy enables element-selective characterization of materials under *in situ/operando* conditions. The information that can be obtained concerns oxidation and spin state as well as atomic coordination. In fact, X-ray spectra are sensitive to almost any modification of the electron density around the analyte atom, *i.e.* the element to be spectroscopically investigated. Functional materials often contain several active sites and are thus composed of many analyte atoms. Ideally, all active elements are studied in one experimental session. The energy range between 1.5 and 4.0 keV (tender X-rays) requires vacuum conditions rendering *in situ/operando* experiments considerably more difficult. It covers the K-edges of Al, Si, P, S, Cl, K and Ca, the L-edges of 4d transition metals and the M-edges of actinides. 4d transition metals and actinides can also be measured in the hard x-ray range but the smaller lifetime broadening and favorable selection rules to probe the valence orbitals directly make the tender X-ray range interesting also for those elements. X-ray spectroscopy beamlines often feature a secondary monochromator that analyses the fluorescence emitted from the sample additional to the primary monochromator that selects the energy of the photon incident on the sample. X-ray emission spectroscopy (XES) in combination with X-ray absorption spectroscopy (XAS), photon-in/photon-out spectroscopy, can provide sharper spectral features and allows studying the occupied and unoccupied density of electronic states thus providing a wealth of information. Furthermore, such an instrument often dramatically improves the data quality by suppressing most unwanted X-ray events and thus minimizing the background. This is particularly relevant for high entropy systems with low analyte concentration and high fluorescence background.

With the energy transition the requests for *in situ* and *operando* X-ray spectroscopy studies of materials has dramatically grown and with them the need for sample environments that truly reproduce laboratory conditions at the X-ray beamline. The presentation will outline some fundamental aspects of advanced X-ray spectroscopy and present examples in catalysis research.

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Pieter Glatzel is an expert for core hole spectroscopy to study electronic structure. He is currently leading the Electronic Structure, Magnetism and Dynamics Group at the European Synchrotron Radiation Facility in Grenoble, France. He received his PhD from Hamburg University and worked at the University of California at Davis, the Lawrence Berkeley National Laboratory and Utrecht University. He has been pioneering various X-ray spectroscopy techniques and developed methodologies for the interpretation of X-ray spectra. His work as spectroscopist has led to many collaborations in the field of materials science including heterogeneous catalysts, coordination chemistry and biocatalysis and luminescent materials. Pieter received the Farrel Lytle young scientist award and was chair of the International X-ray Absorption Society.

KN-3: Asking Ligands to Lend a Hand: Rational Design of 3d Metal-Based Catalysts

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Abstract

The lack of well-defined metal-precursors, kinetic lability, metal redox and controlling selectivity are the key challenges in the development of 3d metal based catalytic systems. Ligand design can play an important role in overcoming these difficulties. In this talk, I will discuss the use of secondary coordination sphere interactions for the development of Fe based oxidation catalyst for the Wacker process. Further, judicious installation of O center on the ligand scaffold to achieve hydroboration reactions on Mn center will be discussed. Further, new ligand scaffolds that display metal-ligand cooperation will be disclosed.

Recent Publications

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2. Chem. Eur. J., **2024** (DOI:10.1002/chem.202400337)
3. Green Chemistry, **2023** (doi:10.1039/D3GC00672G)
4. Chem Eur J, **2023**, (doi:10.1002/chem.202301758)
5. Chem Comm, **2023** (doi:10.1039/D3CC01251D)
6. ACS Catal., **2022** (doi:10.1021/acscatal.2c05086).

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Jitendra Bera received Ph. D. from Indian IISc, Bangalore in 1999. After a couple of postdoctoral stints, he joined the faculty at IIT Kanpur in 2003, where he is currently serving as Chair Professor. He is elected fellows of three National Science Academies (FASc, FNASc, FNA) and recipient of J C Bose National Fellowship. His research in the field of Organometallic Chemistry has earned him several awards and recognitions including Outstanding Investigator Award by DAE, Swarnajayanti fellowship (2009) by DST and Silver medal (2020) and Bronze medal (2012) by Chemical Research Society of India (CRSI). He received C. N. R. Rao National Prize (2018) in Chemical Sciences. He is currently serving as an Associate Editor, Applied Organometallic Chemistry (Wiley), Member: Editorial Advisory Board of Organometallics (ACS), Dalton Transactions (RSC). Bera's research interests span synthetic, structural and mechanistic organometallic chemistry and addresses energy, environmental and sustainability aspects of chemical synthesis.

KN-4: Metal-Free Catalysis for CO₂ Functionalization

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Abstract

In recent years, metal-free catalysis has gained recognition as a sustainable approach due to its cost-effectiveness and environmentally friendly nature. The metal-free catalytic reduction of CO₂ offers an affordable and efficient alternative for chemical processes, utilizing abundant, non-toxic reagents while minimizing the carbon footprint.

In this talk, I will present our recent efforts in developing highly reactive nucleophiles as metal-free catalysts for the reductive functionalization of CO₂. I will focus on the discovery of new reactions with CO₂ which can significantly extend the scope of CO₂ utilization. In particular, I will discuss a recently developed reaction in our laboratory on the S-formylation of thiols using CO₂. Currently, no known chemical process mimics the enzymatic S-formylation of thiols using CO₂. We have developed the first chemical process to produce S-formyl thiols from CO₂ under ambient, metal-free conditions. Through this method, we also synthesized ¹³C-labeled formyl coenzyme A from ¹³CO₂ for the first time. Additionally, we have created a one-pot formylation/olefination strategy to synthesize olefins (vinyl sulfides) using our S-formylated product under entirely metal-free conditions in the presence of CO₂.

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Swadhin Mandal is a professor at the Indian Institute of Science Education and Research (IISER) in Kolkata. Earlier, he was head of the Department of Chemical Sciences at IISER Kolkata from 2018 to 2020. He earned his BS and MS degrees from the University of Kalyani. In 2002, he received his doctorate from the Indian Institute of Science, Bangalore, under the supervision of Prof. S. S. Krishnamurthy. He then worked as a postdoctoral fellow with Prof. Robert C. Haddon at the University of California, Riverside, USA and as an Alexander von Humboldt fellow with Prof. Herbert W. Roesky at the University of Göttingen, Germany. He joined IISER Kolkata as an assistant professor in 2007 and was promoted to full professor in 2018. His current research interests include metal-free catalysis with reactive electron-rich main group species for discovering new chemical transformations of CO₂ and electron transfer catalysis with small molecules in various organic transformations. He is the recipient of the Shanti Swarup Bhatnagar Prize in Chemical Science in 2018, and the Friedrich Wilhelm Bessel Research Award by the Alexander von Humboldt Foundation, Germany, in 2020. He is a fellow of the Indian National Science Academy (FNA) and the Indian Academy of Sciences (FASc). He has been a visiting professor at IIT Bombay, Erna and Jacob visiting professor at Weizmann Institute of Science, Israel, Rutgers University, USA, and Paul Sabatier University, France.

KN-5: Light-Harvesting Organic Heterostructures

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Abstract

Low-dimensional heterostructures that combine two or more optically or electronically complementary organic semiconductors offer an exciting class of organic materials with novel physicochemical properties at their junctions. These organic heterostructures hold great promise for applications in energy conversion, optoelectronics, and catalysis. They provide the much sought after soft and flexible analogue to the well-studied inorganic heterostructures. However, the design and construction of purely organic low-dimensional heterostructures are still in their infancy, as they require precise control over multiple components at all hierarchical levels of structural organization. The bottom-up approach of molecular self-assembly due to its modular approach and the potential to go beyond the limits and functionality of top-down techniques, would be the best practical approach for building a wide variety of functional, complex and ordered organic nanostructures. How far can we push self-assembly? is recognized as one of the big scientific questions in materials science and the next grand challenge will be to assemble and integrate multiple building blocks in a perfect fashion to construct multi-component organic heterostructures.

Over the last decade, our group has mastered the precision molecular self-assembly of organic π -conjugated systems, achieving unparalleled control over dimensions and narrow dispersity. This success is achieved by a deep understanding of the kinetics and thermodynamics governing self-assembly processes. Positioned at the tip of the next level of complexity, we have recently attempted the construction of a diverse array of nascent organic heterostructures—ranging from axial and orthogonal to core-shell and branched topologies—by controlling the molecular self-assembly and integration of electronically complementary π -conjugated organic building blocks. The talk will delve into our ongoing efforts in this direction.

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Subi George is currently leading a supramolecular chemistry group at the New Chemistry Unit of JNCASR, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India. Currently, He is also the Chair of New Chemistry Unit and also the Associate Editor of Chemical Science (RSC). His current research interests focus on Functional Supramolecular Polymers, Living and Non-equilibrium supramolecular polymerization, Supramolecular Chirality and Organic Phosphors. He is the recipient of Shanti Swarup Bhatnagar (SSB) Prize for Science and Technology in Chemical Sciences Category for the year 2020. He is also the recipient of Swarnajayanti Fellowship from Department of Science and Technology of Government of India (2017), Asian Photochemistry Association (APA) Young Scientist award (2015), NASI-SCOPUS Young Scientist Award in Chemistry (2015), Chemical Research Society of India Bronze Medal (2015) and Materials Research Society of India Medal (2013). In 2019, he has been elected as the Fellow of Indian Academy of Sciences (FASc) and in 2023 he is elected as Fellow of Indian National Science Academy (FNASc). In 2021, he received CNR RAO National Prize for Chemical Research from CRSI. He is currently the member of Editorial Advisory Boards of JACS, Material Horizons, Organic Materials, ACS Materials-Au, PCCP and Chemistry Asian Journal.

KN-6: Thermal Topochemical Polymerization Reactions: Challenges and Opportunities

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Abstract

Topochemical reactions, the reaction between pre-organized reacting motifs in the crystal lattice, are attractive as they do not require solvents, catalysts and other special reaction conditions for the reaction and provide products in pure form. Also such reactions provide basic understanding about mechanistic and geometrical details about a reaction.¹ We have employed thermal Topochemical Azide–Alkyne Cycloaddition (TAAC), Topochemical Ene-Azide Cycloaddition (TEAC) and Topochemical Diels–Alder Cycloaddition (TDAC) reactions to synthesize various biopolymer mimics. We have exploited hydrogen bonding for the self-assembly of monomers in solid to pre-organize the reacting motifs. Lattice controlled polymerization/oligomerization reaction of such self-assembled (pre-organized) monomers gave various biopolymer mimics. By applying this methodology, we have topochemically synthesized monodisperse glycopolymers, oligosaccharide mimics, DNA analogs and polypeptides.^{2–14} In this talk, the design and execution of such topochemical syntheses and their possible applications will be discussed.

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KN-7: Phonon-Glass Electron-Crystal like High Performance Thermoelectrics

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Abstract

Achieving glass-like ultra-low thermal conductivity in crystalline solids with high electrical conductivity, a crucial requirement for high-performance thermoelectrics, continues to be a formidable challenge. A careful balance between electrical and thermal transport is essential for optimizing the thermoelectric performance. Despite this inherent trade-off, the experimental realization of an ideal thermoelectric material with a phonon-glass electron-crystal (PGEC) nature has rarely been achieved. We demonstrated high thermoelectric performance with a near room-temperature figure of merit, $zT \sim 1.5$ and a maximum $zT \sim 2.6$ at 573 K by optimizing atomic disorder in Cd doped polycrystalline AgSbTe_2 .^{1,2} Cadmium doping in AgSbTe_2 enhances cationic ordering, which simultaneously improves electronic properties by tuning disorder-induced localization of electronic states and reduces lattice thermal conductivity via spontaneous formation of nanoscale ($\sim 2\text{-}4\text{ nm}$) superstructures. Recently, we showed that isovalent Yb-doping induced enhanced atomic ordering decreases the overlap between the hole and phonon mean free paths and consequently leads to a PGEC-like transport in AgSbTe_2 . A twofold increase in electrical mobility is observed while keeping the position of the Fermi level nearly unchanged and corroborates the enhanced crystalline nature of the AgSbTe_2 lattice upon Yb doping for electrical transport, which leads to $zT \sim 2.4$ at 573 K. These achievements highlight the potential of our approach in enhancing the thermoelectric performance of the material by tuning its inherent atomic disorder which can be applicable to other thermoelectric materials.⁴

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KN-8: Selectivity in CO₂ Reduction

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Abstract

The electrocatalytic CO₂ reduction reaction (CO₂RR) to generate fixed forms of carbons that have commercial value is a lucrative avenue to ameliorate the growing concerns about the detrimental effect of CO₂ emissions as well as to generate carbon-based feed chemicals, which are generally obtained from the petrochemical industry. The area of electrochemical CO₂RR has seen substantial activity in the past decade, and several good catalysts have been reported. While the focus was initially on the rate and overpotential of electrocatalysis, it is gradually shifting toward the more chemically challenging issue of selectivity. CO₂ can be partially reduced to produce several C₁ products like CO, HCOOH, CH₃OH, etc. before its complete 8e⁻/8H⁺ reduction to CH₄. In addition to that, the low-valent electron-rich metal centers deployed to activate CO₂, a Lewis acid, are prone to reduce protons, which are a substrate for CO₂RR, leading to competing hydrogen evolution reaction (HER). Similarly, the low-valent metal is prone to oxidation by atmospheric O₂ (i.e., it can catalyze the oxygen reduction reaction, ORR), necessitating strictly anaerobic conditions for CO₂RR. Not only is the requirement of O₂⁻ free reaction conditions impractical, but it also leads to the release of partially reduced O₂ species such as O₂⁻, H₂O₂, etc., which are reactive and result in oxidative degradation of the catalyst. In this presentation, mechanistic investigations of CO₂RR by detecting and chemically trapping and characterizing reaction intermediates are used to understand the factors that determine the selectivity in CO₂RR. The spectroscopic data obtained from different intermediates have been identified in different CO₂RR catalysts to develop an electronic structure selectivity relationship that is deemed to be important for deciding the selectivity of 2e⁻/2H⁺ CO₂RR. The roles played by the spin state, hydrogen bonding, and heterogenization in determining the rate and selectivity of CO₂RR (producing mostly only CO, HCOOH, CH₃OH, CH₄ or C₂H₆) are discussed using examples of iron porphyrin bioinspired artificial mimics. In addition, strategies are demonstrated where the competition between CO₂RR and HER as well as CO₂RR and ORR could be skewed overwhelmingly in favor of CO₂RR in both cases.

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Abhishek obtained his undergraduate degree from the Presidency College, Calcutta and his PhD from Stanford University, CA, USA. He joined IACS in June 2009 as an Assistant Professor and is currently serving as a senior Professor at the school of chemistry. He is the recipient of the American Chemical Society Division of Inorganic Chemistry Young Investigator Award, Society of Porphyrin and Pthalocyanine Young Investigator Award, James Hoeschele award from the Asian Biological Inorganic Chemistry, and Society of Biological Inorganic Chemistry Emerging Investigator Award. India. He has been a Young Associate of the Indian Academy of Science, a CRSI Bronze medal awardee and a SERB-STAR fellow. He is an elected fellow of Indian Academy of Science (FASc), Bangalore, National Academy of Sciences (FNASc), India and the National Academy of Sciences (FNA). His current area of research involves development of homogeneous and heterogeneous catalysts for sustainable energy and clean environment. A combination of synthesis, self-assembly, spectroscopy, electrochemistry and electronic structure calculations are used to attain these research goals. He has served the international editorial advisory boards of Chemical Reviews, Chemical Communications, Inorganic Chemistry, Journal of Biological Inorganic Chemistry and ACS Catalysis. Currently he is an associate editor of ACS Catalysis. He is serving as the elected president of Asian Biological Inorganic Chemistry (AsBIC).

KN-9: Decoding Photo-accumulation of Charge in Ionic Carbon Nitride - Applications for Solar Battery and Dark Photo-catalysis

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Abstract

Integrating solar energy capture and storage directly into an electrical form in a single material presents a promising strategy to address the intermittency aspect of solar power. In recent years, the ionic carbon nitride (F-PCN) has been showcased to have a unique ability to photo-accumulate charge (PAC), which was subsequently utilized for dark photo-catalysis and solar battery applications. However, the understanding of underlying chemical and structural factors governing PAC formation in F-PCN remains unclear. The work that will be discussed aims to establish a structure-property relationship for F-PCN by showcasing the detailed structure of its ground and PAC state using a combination of *ex-situ* and *in-situ* spectroscopic techniques along a computational study. The findings reveal the crucial structural features (such as $\text{--N-C}\equiv\text{N}$) and mechanisms that enable photo-accumulation of charge in ionic carbon nitride. Additionally, the study proposes a donor-acceptor model to explain PAC behavior, offering a unified understanding of F-PCN's dual functionality and valuable guidance for designing advanced energy materials, particularly for applications in dark photo-catalysis and solar batteries.

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Deepa Khushalani received her Phd from University of Toronto in 1998 and subsequently worked as a Postdoc in University of Bristol. From 2001-2004 she worked as a lecturer in University of Kent before returning to India in 2004 where she has been working at TIFR, she is currently a Professor in Materials Chemistry. Her area of specialization involves materials chemistry with emphasis on exploiting alternate sources of clean energy involving photovoltaics and energy storage devices. Her group also works on drug delivery devices, photocatalysis and electrocatalysis. She is the recipient of the DST Nanoscience Young Investigator award 2016 and the CRSI Bronze Medal in 2018. She is a Fellow of Royal Society of Chemistry (FRSC), Editorial Board Member of ACS Energy & Fuels.

KN-10: Catalysis for Sustainable and Circular Chemistry

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Abstract

Achieving more sustainable chemical processes and enabling a circular economy are major scientific goals, which play significant roles in the implementation of resource- and cost-efficient chemical industry as well as the advancement of society with respect to health, energy, and the environment. In this regard, the valorization of more abundant feedstocks, renewable resources, and waste-materials to produce value-added products is of prime importance. In order to achieve these goals, the development and applicability of suitable catalytic processes is crucial. The major challenge in catalysis is to create ‘ideal’ catalysts which should be more stable and easily recyclable as well as highly selective and active. Consequently, in the talk the design and catalytic applications of specific NPs and SACs as well as molecularly defined complexes for sustainable synthesis of essential fine and bulk chemicals as well as molecules used in life science applications will be presented. Next, catalytic applications on the valorization of renewable feedstocks (biomass and CO₂) and recycling/upscaling of waste-plastics for enabling sustainable and circular chemistry will be discussed.

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The research group of Prof. Jagadeesh Rajenahally works on sustainable catalytic processes for the synthesis of essential fine and bulk chemicals, pharmaceuticals, and agrochemicals as well as for the valorization of renewable feedstocks (biomass and CO₂) and circular chemistry for enabling circular economy (valorization of waste-materials, plastics-waste and use them as resources/feedstocks for chemicals upgrading). Important works of his group have been published in notable journals: 3 research papers in *Science*, >10 research papers in *Nature Publishing Group Journals* and 3 research papers in *Cell Press Journals*. Interestingly, key work related to the development of iron-based nanocatalysts for an industrially important hydrogenation process has been highlighted and featured on the ‘Cover of *Science*’. In addition, important works are highlighted in *Science*, *Nature*, *Chemical & Engineering News (C&EN)* *Chemistry World*.

KN-11: Reticular Chemistry: From Covalent Organic Frameworks to Porous Crystalline Nitrogen Doped Graphite

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Abstract

Covalent Organic Frameworks (COFs) represent a novel class of highly porous, crystalline polymers with uniformly ordered pore channels. Despite their extensive use for storing various molecular species such as gases, nanoparticles, enzymes, and drugs, the potential of their ordered pore channels for molecular separation still needs to be utilized. Recent advances in Reticular Chemistry have led to the development of Covalent Organic Nanotubes (CONTs), which extend the principles of COF design into one-dimensional architectures. These CONTs, formed by linking molecular building blocks in a reticular fashion, offer unique properties such as tunable pore sizes and enhanced stability, making them promising candidates for molecular separation, catalysis, and nanofiltration applications. Integrating reticular chemistry in one dimension opens new avenues for designing functional materials with precise control over their structural and chemical features. Our findings highlight that COMs and CONTs have significant potential to address some of the world's most challenging separation problems, including wastewater treatment and drug recovery in the pharmaceutical industry. We could combine 2,4,6-trimethoxybenzene-1,3,5-tricarbaldehyde with benzene 1,4-diamines, culminating in the formation of two-dimensional materials reminiscent of fully aromatic structures like graphite. The newly developed covalent organic frameworks (COFs)-resemble N-doped graphite and display high crystallinity. Additionally, their N₂ adsorption isotherms confirm the presence of permanent porosity. These porous aromatic NPH materials, with their unique combination of graphite-like connectivity and COF-like porosity, hold significant promise for electrochemical energy applications.

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KN-12: Role of Materials in Scale-up of Renewable Energy and CCUS for NetZero India by 2070. How do we Make it Sustainable?

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Abstract

Global CO₂ emission has touched ~40 billion tons per year, and despite all the talk about NetZero CO₂ emission, the rate of CO₂ emission is expected to stay at the current level for few years. Currently, India contributes roughly 10% in total global CO₂ emission, however, this share is growing every year. While role of solar, wind, hydro/waves, hydrogen etc. (perhaps nuclear as well) is acknowledged, current energy need, and proposed GDP growth of a developing country like India could not be achieved without also ensuring implementation of Carbon Dioxide Capture Utilization and Sequestration (CCUS). CCUS is essentially a three-step process, i) Capturing or separating the CO₂ from its associated gases, ii) Transporting the captured, relatively purer CO₂ (from step-i) to the utilization site where part of the CO₂ could be processed for its utilization, and iii) Majority of the CO₂ which could not be converted (in step-ii) has to be transported and sequestered for geological timescale. Utilization of renewable energy (RE) and CCUS would deliver the desired outcome if we optimize the entire process for NetZero CO₂; this presentation will briefly explain the challenges and available solutions, and what are the right questions one should be asking for achieving net zero in terms of CO₂ emission.

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KN-13: Ligand-Enabled Redox Gold Catalysis

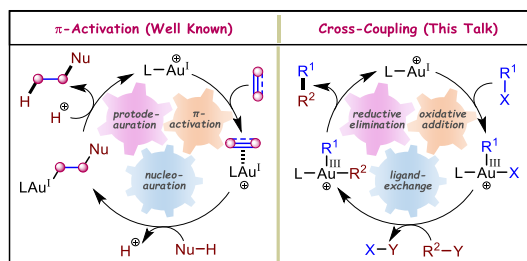
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Abstract

Traditionally, gold complexes have been recognized as Lewis acid catalysts for the activation of C-C multiple bonds (Scheme, LHS). Over the years, there has been a considerable shift, and Au(I)/Au(III) redox catalysis is now recognized as an established technique for achieving cross-coupling reactivities (Scheme, RHS). The pioneering work by Zhang and Toste group revealed the role of external oxidants to overcome the high redox potential of Au(I)/Au(III) couple ($E^0 = +1.41$ V) and to facilitate two-electron redox cycle in gold catalysis. Later, the Glorius group introduced the merged gold/photoredox strategy to circumvent the need for a stoichiometric oxidant in these processes. Recently, ethynylbenziodoxolones (EBXs) have also been used for accessing redox gold catalysis serving dual role as oxidant and alkyne surrogate. All the above strategies were not amenable to the use of aryl halides, and thus their use in gold-catalyzed cross-coupling reactions remained forbidden. In recent years, ligand-enabled gold-catalyzed organic reactions have emerged as a valuable tool, allowing for the use of aryl halides as cross-coupling partners. In this talk, I will discuss our most recent work on alkene functionalization employing cross-coupling reactivities.



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Prof. Nitin Patil is a distinguished researcher whose work focuses on the unique reactivity of gold complexes in catalysis. His research group explores gold's unparalleled ability to function as a π -Lewis acid for the selective activation of carbon-carbon multiple bonds, leading to the development of innovative catalytic transformations. These efforts aim to overcome limitations in conventional transition metal catalysis and address challenges in organic synthesis through cascade reactions, oxidative gold catalysis, and hybrid gold/metal or gold/organo-catalysis. Dr. [Name]'s groundbreaking work has potential applications in both materials and biological sciences, and he continues to push the boundaries of chemical reactivity. His accolades include the CNR Rao National Prize for Chemical Sciences (2024), J.C. Bose National Fellowship (2023), and SERB-TETRA Technology Translation Award (2023). He is a Fellow of several prestigious scientific academies, including the Indian National Science Academy (FNA), The Royal Society of Chemistry (FRSC), The National Academy of Sciences (FNASc), and the Maharashtra Academy of Sciences (FMASc). Among his other recognitions are the SERB Distinguished Investigator Award (2018), Chemical Research Society of India (CRSI) Bronze Medal (2018), and Indian National Science Academy (INSA) Young Scientist Medal (2010).

KN-14: Determination and Perturbation of Electron Potentials in Solid Catalysts: Bridging the Gap among Thermal-, Electro-, and Photo-Catalysis

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Abstract

The growing demand for higher catalytic efficiency requires researchers to revisit the catalytic systems and contribute to their innovation. Electrochemical means has gradually shown its high capability for operando catalyst characterization and further promotion of thermal- and photo-catalytic activity when (photo)catalysts are fabricated into a working electrode (WE).¹ The open-circuit potential (OCP) of a catalyst, i.e., without current flow, shows dependence on the identities and coverages of adsorbates on its surface, which subsequently regulates the catalytic activity. In this configuration, the mixed potential theory (MPT) to elucidate catalysis involving multiple reactants, separating a reaction into two independent electrochemical half-reactions that are coupled together by internal charge transfer through the catalyst. Furthermore, external potentials can also be applied to the catalysts in pursuit of promoted catalytic performance, known as electrochemical promotion of catalysis (EPOC). In this presentation, four energy-conversion reactions are selected as examples: Namely, aerobic oxidation/hydrogenation of hydroquinone/benzoquinone redox couple over Pt-based catalysts, aqueous formic acid dehydrogenation (FAD) over supported Pd-based catalysts,² aqueous aerobic CO oxidation over supported metal catalysts,³ and photocatalytic overall water splitting under UV-irradiation.^{4,5} By employing operando OCP monitoring and in situ spectroscopic techniques, quantitative coverage-potential-performance correlation was attempted to obtain. The universality of such electrochemical methodology as well as the conditions when MPT is applicable are also discussed. The findings in this study contribute to bridging the gap between thermal-, electro- and photo-catalysis and represent the potential of electrochemical tools for elucidation and promotion of thermal- and photo-catalytic reactions.

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Dr. Kazuhiro Takanabe is Professor in the Department of Chemical System Engineering at The University of Tokyo since 2018. He previously worked at the University of Twente in the Netherlands (2002-2004), at the University of California at Berkeley (2006-2008), at the University of Tokyo (2008-2010), and at King Abdullah University of Science and Technology (KAUST) (2010-2018). He is currently Editor of the Journal of Catalysis since September 2017. He has been assigned as a team leader of JST-GteX Water Electrolysis WInG project (2023-2027), which involves 24 laboratories across Japan, targeting to reduce the cost of green hydrogen production.

His research topics address the important dynamic transition of energy systems using conventional fossil fuel to new renewable energy; including electrocatalysis for water splitting and CO₂ reduction, photocatalysis for water splitting, natural gas conversion, metal cluster chemistries, and ammonia synthesis via innovative technology. His research group not only develops novel catalysts but also studies kinetics and reaction mechanisms at molecular level. The research aims to bridge the gap among the fields of thermal-, electro-, and photo-catalysis, which are addressed through world-wide collaborations to achieve practical industrialization.

KN-15: Introducing the Iliad – The First Fully Integrated Advanced Analytical L-shaped (S)TEM

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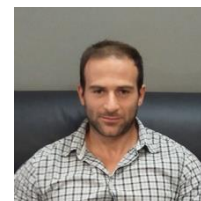
Abstract

Over the last decades we have witnessed a tremendous development in advanced transmission electron microscopy. To name a few, probe correctors have become more powerful and now in combination with ultra-brightness electron sources 60 – 70pm spatial resolution in STEM can be routinely reached with nearly 1nA probe current, improvements in energy resolution have led to phonon spectroscopy, EDS detector systems have become 6x more efficient and sensitive with the latest generation leading to low-dose data collection and in-situ analytical studies, detectors are now capable to count electrons dramatically reducing the contribution of instrumental noise and that has led to the revolution in cryo-EM.

Very recently with the market introduction of the Iliad (S)TEM microscope platform, Thermo Fisher Scientific has brought, for the very time, full microscope hardware and software integration that now extends and includes the Iliad EELS spectrometer and energy filter and the NanoPulser the Ultrafast Electrostatic Beam Blanker ESBB. Multimodal integration of EELS, EDS and the NanoPulser ensures the most advanced and effective electron dose optimization strategies. EELS data collection is extended with the ease-of-use of Velox software ecosystem making the most challenging experiments now accessible to every user including novices. Nearly every component in the Iliad platform can be fully accessed via Python scripting using Autoscript and that opens the possibility of creating new data collection workflows as well as the adoption of Artificial Intelligence based data collection and processing strategies.

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Paolo Longo is the Director of Product Marketing in the High-End TEM group within the Material Science Business Unit

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Prior to joining Thermo Fisher Scientific, Paolo was at Gatan Inc. for over 10 years in various roles supporting initially the GIF (Gatan Imaging Filter) product line and lately all TEM and SEM products for both Gatan and EDAX as Director of Global applications. During his time at Gatan, Paolo was key to promote and successfully establish direct detection solutions for EELS data collection in the analytical TEM market.

Paolo has a rich background in analytical (S)TEM which also helps to strengthen the core applications expertise of the entire TEM product portfolio within Thermo Fisher Scientific. In 2008, Paolo obtained his PhD in Physics from the University of Glasgow (UK), where he worked on the chemical and compositional characterization of semiconductor transistors using a combination of EELS STEM based techniques.

KN-16: Novel Adsorbents Derived from Bio-Waste for Water Treatment

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Abstract

This presentation focusses on the development of adsorbent materials derived from bio-waste for the efficient removal of aqueous pollutants. Three distinct composites were developed, namely nZVI/graphene by phytochemical route, biochar/CeO₂ from coconut shells, and Ni/NiO decorated biochar from chitosan. These materials demonstrated good performance in removing heavy metals like chromium, arsenic(V), and several dyes from aqueous solutions. The nZVI/graphene composite achieved complete removal of Cr(VI) in a short period of time, with a maximum adsorption capacity of 46 mg/g. The biochar-cerium oxide composite removed 99% of As(V) with a high adsorption capacity of 61 mg/g. The Ni/NiO biochar composite showed 82% removal of methyl orange, with an adsorption capacity of 140 mg/g. All three materials exhibited rapid adsorption kinetics, following pseudo-second-order models, and adsorption isotherms fit well with the Langmuir model. Thermodynamic studies revealed spontaneous and exothermic adsorption processes for all composites. The use of phytochemical route for synthesizing these adsorbents highlights the preparation of sustainable and eco-friendly sorbents for water treatment applications.

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Prof. Subrahmanyam's research centers on advanced materials for harvesting, CO₂ conversion to value added chemicals.. His group's work in Plasma catalysis, Photo-/electrocatalysis, Hydrogen Storage, and Surface chemistry exemplifies how fundamental science drives innovation in clean energy and sustainable chemical production. Their focus on cutting-edge nanocatalytic processes offers promising solutions for energy transformation and storage, linking basic science to practical applications. He obtained his PhD degree in Chemistry from the Indian Institute of Technology Madras in 2003. From 2003 to 2007, he was a postdoctoral fellow at the École polytechnique fédérale de Lausanne, Switzerland. He started his academic career as an assistant professor at the National Institute of Technology Trichy, India. In 2009, he moved to the Indian Institute of Technology Hyderabad as an assistant professor, where he is currently a professor. He held several administrative responsibilities like the Dean Academics, Director (i/c), Chairman JEE Adv/GATE, Coordinator PMRF, etc.

KN-17: Buckling and Defects in Two - Dimensional Atomically Thin Monolayers

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Abstract

Graphene has emerged as one of the most fascinating areas of research in condensed matter and materials science. Apart from graphene, several other 2D analogues like silicene, phosphorene, MXenes, MoS₂, germanene have been recently isolated and characterized. One unifying theme among these new materials is that unlike graphene, they are non-planar. The mode and measure of the buckling (puckering) from planarity depends on the local electronic structure. The effects of such ripples are manifold particularly in its local reactivity to halogens and hydrogens along the more $\sim sp^3$ atoms. Pseudo Jahn-Teller (PJT) distortions is shown as a central unifying concept that explains the overall structural preferences of these systems. The extent of buckling also leads to interesting and emerging phenomenon like phase-transitions into Topological Insulators from normal semi-metal due to spin-orbital coupling (SOC). The effect of PJT in bestowing structural diversity and novel electronic and spin phases in 2D-monoatomic layers will be discussed in this lecture.

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Prof. Ayan Datta, after his Ph.D. in 2007, worked as a postdoc in USA for a few years before starting his own independent group at IISER TVM. In 2012, he moved to IACS, and his group is working on the development of computational models for energy and environment. He is the recipient of the INSA Young scientist award and BM Birla Prize in Chemistry. He was also awarded the distinguished investigator award (DIA) by DST-SERB in 2017. He was awarded a Bronze medal by the Chemical Research Society of India (CRSI), India.

KN-18: Navigating the Expected and Unexpected Twists and Turns of Lead Optimization: The Discovery of Clinical Candidate for the Treatment of Parkinson Disease

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Abstract

The 'one drug, multiple targets' concept has gained attention of both the academic and the pharmaceutical industry in recent years. To achieve such goals concept of molecular hybridization was put forward wherein two or more distinct pharmacophores are covalently linked into a single molecule.^{1,3} The development of such molecular frameworks with synthetic selectivity and economic viability is still a challenging task for the pharmaceutical industry. Drugs developed through this approach can be used for the cure of infectious diseases where treatment is limited to few drugs and the known drugs have limitations such as toxicity, pharmacokinetics, pharmacodynamic and drug resistance. The benefit of using molecular hybrid is to activate different or same targets by a single molecule, and increase the therapeutic efficacy and to improve the bioavailability. Molecular hybridization approach has resulted many drug candidates with improved activity profile and some of these compounds are in clinical trials.⁴ We have utilized this concept in designing antimalarial molecules and many molecules with aminiquinoline and pyrimidine pharmacophore showed low nano molar activity. Later a massive multi-institutional collaboration was started and over 700 new molecules were studied for Nurr1 activation, a potential target for Parkinson disease model and identified 15 hits out of which 3 compounds have cleared pre-clinical trials and technology has been transferred to NURRON pharmaceuticals for further development.⁵⁻⁸ These molecules activate the Nurr1 enzyme which is essential for the survival of the dopamine neurons, stops the aggregation of α -synuclein protein in the brain, and promotes autophagy. Systematic studies demonstrated that these compounds can cure the Parkinson induced mice model at 5 mg/kg body weight without any toxicity and recently one of the molecule has successfully cleared phase I human clinical trials.

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Prof. Diwan S Rawat, is currently serving as a Vice Chancellor of Kumaun University and his research interests lie in the area of drug development and catalysis for industrial applications. Prof. Rawat has published over 170 research papers, authored a book, seven book chapters, and fourteen patents to his credit. His research work has been cited over 7350 times with h-index of 50 and i-10 index of 137. One of his compounds has cleared phase I human clinical trials for the Parkinson treatment. Prof. Rawat has supervised 28 PhD students. He was elected as President of Chemical Sciences Section of Indian Science Congress (2019-20) and he is a Visiting Professor at Japan Advanced Institute of Science and Technology. Prof. Rawat is a recipient of many awards such as Vasvik research award (2022), ISCB Excellence award in drug discovery (2022), Excellence award for exemplary services, University of Delhi (2021). Prof. Rawat is an elected Fellow of National Academy of Sciences and Fellow of Royal Society of Chemistry.

KN-19: Dynamic Molecular Crystals

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Abstract

High crystallinity, although desired in materials for a wide range of high-performance engineering applications, generally comes with undesirable attributes such as high brittleness and fragility.¹ This makes crystalline materials incompatible with many future technologies, such as flexible devices and soft-robotics. Recent progress in crystal engineering has brought into light many possible opportunities to address these issues, enabling the design of adaptive crystalline materials that respond to external stimuli with exceptional qualities.¹⁻⁷ For instance, crystals that bend (elastically or plastically), twist, curl, wind, jump, exfoliate, laminate, and explode, under external stresses, such as mechanical stress, pressure, light, heat, solvent, etc., have been shown. On the other hand, until very recent times, self-healing was observed only in soft and amorphous materials, mostly involving approaches that use chemical reactions, diffusion, solvent, vapor, electricity, etc., with typical healing time scales in minutes to weeks.⁸ A new self-healing mechanism that we recently introduced⁹ enables ultrafast, near 100% autonomous diffusion-less repair in crystalline materials. My talk will cover structure-property correlation in adaptive materials useful for various applications, including barocaloric.

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Dr C Malla Reddy is a Professor at the Department of Chemistry, IIT Hyderabad. Prior to joining IITH in December 2023, he spent about 15 years at the Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Kolkata. He is a recipient of prestigious Swarna Jayanti Fellowship from DST, Govt of India (year 2015) and the elected fellow of the National Academy of Sciences, India. He is the Editor-in-Chief for the journal CrystEngComm published by Royal Society of Chemistry. His research work focuses on the understanding of the structural basis for the mechanical behavior of solid dosage forms, mechanism of mechanically flexible and self-healing functional crystals from the crystal engineering point of view. His group is particularly interested in addressing performance related issues of pharmaceutical solids at particle level using structure-mechanical property correlation, and screening and development of polymorphs and different other solid forms of APIs.

KN-20: Post-Modified Metal-Organic Frameworks for Solar Fuel Production

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Abstract

The much-needed renewable alternatives to fossil fuels can be achieved efficiently and sustainably by converting solar energy to fuels via hydrogen generation from water or CO₂ reduction. Sunlight-driven H₂ production and CO₂ reduction are promising routes for the production of chemical feedstocks as fuel precursors to mitigate the CO₂ concentration in the atmosphere and also to alleviate the global energy crisis.^[1-5] Nature's design of carrying out the photosynthetic redox cycle involving CO₂ and water inspired us to develop highly efficient integrated catalytic systems for artificial photosynthesis. The versatile and highly amenable structural tunability of metal-organic frameworks (MOFs) by post-synthetic modification (PSM) allows for tailoring inherent semiconducting and optoelectronic properties, compared to traditional inorganic semiconductors. Besides, PSM is an excellent choice for introducing a functional photosensitizer into the MOF matrices to galvanize the electronic and optical properties towards photocatalytic H₂O and CO₂ reduction.^[1-3] Our presented results demonstrated an excellent approach to green H₂ production and carbon neutralization for tackling the energy crisis.^[1-6]

My talk will focus on developing integrated photocatalytic systems through post-synthetic modification of MOFs for H₂O and CO₂ reduction.

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Prof. Tapas K. Maji's research centers on the synthesis and structure-property relationships of metal-organic frameworks (MOFs) and porous organic polymers (POPs) at both bulk and nanoscale levels. He has made seminal contributions to MOF and POP research, demonstrating their diverse applications, including cost-effective chemical feedstock separation, geometrical isomer separation, and the removal of toxic metal ions from water. In a pioneering approach, he developed a method of covalently linking light-harvesting units with catalytic moieties in highly porous MOFs, opening new avenues for creating artificial photocatalysts for clean solar fuel production. To further enhance the versatility of these hybrid materials, Prof. Maji's team developed 'soft' gel materials by self-assembling low molecular weight gelators (LMWG) with metal ions, which have applications in catalysis and optoelectronics.

Dr. Maji received the prestigious Shanti Swarup Bhatnagar (SSB) Award in 2019 in Chemical Sciences, along with other honors such as the Materials Research Society of India (MRSI) Medal, the Sheikh Saqr Career Award Fellowship, and the Scopus Young Scientist Award. He is also a Fellow of the Royal Society of Chemistry (RSC) recognized as a Leader in the Field in 2019, and the Indian Academy of Sciences.

KN-21: Green Initiatives for Sustainable Future

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Abstract

The ever-increasing reliance on existing fossil fuels has not only put us to the threshold limit of exhausting non-renewable energies but also caused serious problems in the environment by accumulating significant amounts of greenhouse gas CO₂. A recent study mentioned that about 35.7 Gt of CO₂ will be released into the atmosphere by 2035. The chemical transformation of carbon dioxide into useful products becomes increasingly important as CO₂ levels in the atmosphere continue to rise because of human activities. It emphasizes the necessity of innovations for capturing and utilizing CO₂ to decrease its net emissions or adopting CO₂ reduction technologies. Instead of looking at CO₂ emissions as a threat, it can be viewed as a highly valuable resource/feedstock to transform it into various other chemical forms.

In the 19th Century, the petroleum refining industry has become a foundation of modern society, but it has also led to the global proliferation of greenhouse gas emissions as well as local air pollution from the combustion of fossil fuels. As per the COP26 declaration, India is committed to the NetZero goal by 2070. In line with this oil industry aimed to be net zero by 2050. In this work, various green initiatives of the oil industry are discussed, which support the decarbonization efforts of the oil refining industry.

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Dr. Chiranjeevi Thota is the General Manager at the Corporate R&D Centre of Bharat Petroleum Corporation, India. With over 23 years of research experience in petroleum refining, petrochemicals, biofuels, and fuel additives, his expertise spans refinery and petrochemical catalysts, alternate fuels, and C1 chemistry. He holds a PhD from the Indian Institute of Petroleum, Dehradun, and has received post-doctoral offers from Leipzig University, Germany, and Hokkaido University, Japan. Since joining Bharat Petroleum in 2001, he has contributed significantly to research, with 91 published papers, 2 book chapters, and 52 patents.

Dr. Thota has received numerous honors, including the Asian Oil and Gas Award (2024), CII Best Practices Award (2023), and Golden Peacock Eco-Innovation Award (2021). He has been recognized for his innovative contributions to sustainability and green processes, winning multiple awards from FICCI, CII, and Green Tech. His achievements highlight his leadership in advancing environmentally friendly technologies in the petrochemical sector.

KN-22: Importance of CCUS in Indian Steel Industries: Roadmap for Carbon Neutrality

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Abstract

In India, nearly 2.7 billion tons of CO₂ is produced annually, accounting for around 7% of total global emissions. The iron and steel industries are among the largest industrial emitters of CO₂. To decarbonize the steel sector, approximately 2.5 to 3.0 tons of CO₂ per tonne of crude steel produced need to be abated. According to the World Steel Association (WSA), there is no single solution for CO₂-free steelmaking, and a broad portfolio of technological options are required.

The approaches to reducing CO₂ emissions in the steel industry can be categorized in two ways. First, CO₂ emissions can be minimised by reducing the use of carbon with alternative green reductants, a process known as Carbon Direct Avoidance (CDA). In CDA, hydrogen or hydrogen-bearing gases such as syngas and methane can be used as alternative reductants in blast furnaces. In the CDA route, apart from water electrolysis, generation of hydrogen/ syn-gas from biomass gasification is currently explored by several steel industries as the carbon footprint of the associated process is much less compared to water electrolysis. Second, CO₂ can be captured from steel mill off-gases and then stored or converted into value-added products (such as polycarbonate, syn-gas, methanol, ethanol etc.), a process commonly referred to as CO₂ capture, utilization, and sequestration (CCUS). However, the main challenges of any CO₂ utilization routes are high energy demand, requirement of green hydrogen/ green electricity, and large area requirement. Presently, a huge thrust in research is being given on the resourcing of green hydrogen, using solar energy, geo-thermal energy, and wind energy etc. Considering this, CCUS is going to be an important technology lever for reducing the emissions from existing global blast furnaces, which are expected to remain operational for a significant amount of time in the coming decades. The International Energy Agency (IEA) estimates that CCUS technology must be applied to more than 53% of primary steel production by 2050, equivalent to 700 Mtpa of CO₂, to achieve the Net Zero Emissions scenario.

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Dr Pratik Swarup Dash joined Tata Steel in 2001, after completing MTech in Chemical Engineering and later completed his PhD from IIT, Kharagpur. With an extensive 23-years of research experience in the area of coal beneficiation, coke making, advanced carbon materials, CCUS, and environmental sustainability, he presently serves as the Chief of Coal, Coke & Environment Research at R&D, Tata Steel. Dr Dash has received the prestigious 'Tata Innovista Award' four times, 'Young Metallurgist of the Year Award' in 2007 and 'Certificate of Excellence for R&D in Iron and Steel' in 2021 from Ministry of Steel, Govt. of India. Dr Dash has published more than 100 papers in referred international & national journals of repute and conference proceedings. He has also filed more than 90 Indian patents & PCTs. He is an active member of several national level task forces such as CCUS, R&D and Demonstration, and Biomass Utilization for Green Steel under and Ministry of Steel, Govt. of India. Dr Dash also contributes as an expert panel member of Department of Science & Technology (DST), Govt. of India for roadmap preparation & projects evaluation in the area of CCUS.

KN-23: Utilization of CO₂ in Synergistic Triple Catalysis for Anti-Markovnikov Hydrocarboxylation of Industrial Alkenes

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Abstract

The direct use of CO₂ as a C1 synthon for the construction of new carbon-carbon bonds remains a critical challenge in chemical synthesis.¹⁻³ Carbon dioxide, as a linear molecule with no dipole moment, exhibits high kinetic and thermodynamic stability under most reaction conditions. As a consequence, the activation of CO₂ to form carboxylic acid derivatives traditionally requires highly reactive nucleophiles and/or harsh reaction conditions (Fig. 1a).⁴⁻⁶ In contrast, the single electron activation mode of CO₂ proceeds via the generation of an unstable reactive species, carbon dioxide radical anion (CO₂^{•-}), which could potentially be exploited to harness carboxyl functionalities into a plethora of molecules in both academic and industrial setting (Fig. 1a).^{7,8} The direct utilization of carbon dioxide as an ideal one-carbon source in value added chemical synthesis has garnered significant attention from the standpoint of global sustainability. In this regard, the photo/electro-chemical reduction of CO₂ into useful fuels and chemical feedstocks could offer a great promise for the transition to a carbon-neutral economy. However, challenges in product selectivity continue to limit the practical application of these systems. A robust and general method for the conversion of CO₂ to the polarity-reversed carbon dioxide radical anion, a C1 synthon, is critical for the successful valorization of CO₂ to the selective carboxylation reactions. We demonstrate herein a hydride and hydrogen atom transfer synergy driven general catalytic platform involving CO₂^{•-} for highly selective anti-Markovnikov hydrocarboxylation of alkenes via triple photoredox, hydride, and hydrogen atom transfer catalysis. Mechanistic studies suggest that the synergistic operation of triple catalytic cycle ensures a low-steady state concentration of CO₂^{•-} in the reaction medium. This method using renewable light energy source is mild, robust, selective and capable of accommodating a wide range of activated, and unactivated alkenes. The highly selective nature of the transformation has been revealed through the synthesis of hydrocarboxylic acids from the substrates bearing hydrogen atom available for intramolecular 1,n-HAT process as well as diastereoselective synthesis. This technology represents a general strategy for the merger of in situ formate generation with synergistic photoredox and HAA catalytic cycle to provide CO₂^{•-} for selective chemical transformations.

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Prof. Maiti has an expertise in the broad spectrum of organic chemistry. He is one of the pioneers of distal C-H functionalization of organic molecules via the directing group approach. The C-H functionalization of aliphatic C-H bond is a major challenge in chemistry, his design of the suitable catalyst and the reaction conditions can now lead to products with high efficiency and more importantly with excellent selectivity. His recent contribution to the distinct single metal catalyzed cross-electrophile coupling has the potential to bring a new disconnection to the cross-coupling domain. He is currently focusing the utilization of green-house gases such as CO₂, CO in organic chemistry to synthesize important organic products using mild reaction conditions at room temperature.

KN-24: Photoredox Organic Transformations in Water using Host-Guest Charge Transfer Chemistry

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Abstract

Enzymes are proteins that catalyze non-spontaneous organic reactions in physiological conditions. Remarkably the water-insoluble organic substrates are usually encapsulated in hydrophobic protein cavities, which constitute reaction hotspots in enzymes. We have devised a new catalytic photoredox paradigm using water-soluble cationic nanocages [1] that mimic the enzyme cavity while providing a modular host-guest photoactivation strategy. [2, 3,] Through the potent combination of light activation and substrate pre-organization in water, we demonstrate facile yet selective aerobic oxidation of hydrocarbon C-H bonds under ambient conditions using proton-coupled electron transfer (PCET).[2, 4] Additionally sp^2 C-H functionalization [5] and C-C bond formation [6] was demonstrated recently along with usage of aqueous reactivity by a novel cage-trapped Fe(IV)-superoxo complex.[7] Using time-resolved Raman spectroscopy, we show that the water cluster around and inside the nanocage plays a crucial role in driving the PCET chemistry leading to C-H activation. [8] The success of our designed artificial photoenzyme hints at the crucial role of electric fields in driving reactions within nanospaces.

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Prof. Jyotishman Dasgupta received his 5-years Integrated Masters degree in chemistry from Indian Institute of Technology, Kharagpur in 2000. Subsequently he moved to Princeton University as a Hughes Stott Taylor graduate fellow where he carried out his Ph.D. work in the field of oxygenic photosynthesis under the supervision of Prof. G. Charles Dismukes. In 2006, he moved to UC Berkeley where he did his postdoctoral work with Prof. Richard A. Mathies. He joined the Tata Institute of Fundamental Research, Mumbai in 2010, and has been there ever since. The central theme of his research group is to probe dynamical structural events leading to charge generation in molecular materials, in order to fabricate bio-inspired molecule-based devices for photocatalysis and solar electricity generation. He received the 2017 Asian and Oceanian Photochemical Association (APA) Prize for Young Scientist, the 2018 Best Emerging Investigator Award and the 2024 CRS Silver Medal. He has been inducted as a Fellow in the Royal Society of Chemistry as “Leaders in Field”, and has been in the editorial board of the major physical chemistry journals: JPC Letters, Journal Physical Chemistry and Journal of Chemical Physics.

KN-25: Trimetallic Synergy and Defects

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Abstract

The conversion of CO₂ to CO through heterogeneous catalytic processes is a promising strategy for transforming CO₂ into useful products. We designed a catalyst with unique electron density distribution, by leveraging the concepts of defects¹⁻³ and strong metal-support interaction (SMSI)^{2,3}, and discovered Ni-Cu-Zn/CeO₂ catalyst achieving excellent performance. The Ni-Cu-Zn/CeO₂ catalyst showed CO productivity of 49279 mmol g⁻¹ h⁻¹ (i.e., 10,484,894 mmol g_{metal}⁻¹ h⁻¹) at 650 °C, a nine-fold increase as compared to the best-reported catalysts. CO selectivity up to 99% and excellent stability (rate remained unchanged even after 100 h on stream) were also achieved at 500 °C. The reaction can also be carried out at as low as 350 °C with good productivity. Same conventional ceria, same conventional metal sites⁴⁻⁶—so why does this combination of trimetallic sites and defective ceria perform so dramatically? *In-situ* TEM and HERFD-XANES studies provided insights into interaction dynamics and the unique electron density distribution between CeO₂, its defects, and the trimetallic nanoparticles. The catalyst's activity and stability stem from synergistic interactions among Ni-Cu-Zn sites, and their SMSI with defected ceria support. HERFD-XAS confirmed the strong interactions between trimetallic sites and the CeO₂ surface, further corroborated by *in-situ* EELS. The *in-situ* studies (HERFD-XANES & EELS) indicated the key role of oxygen vacancies of defected CeO₂ during catalysis in both activation of the CO₂ molecules and suppression of coke formation. The *in-situ* TEM imaging under catalytic conditions helped in visualizing the movement and growth of active trimetallic sites in real-time, which completely stopped and did not undergo further diffusion and sintering once SMSI was established, even at high temperatures. These findings offer a novel approach to catalyst design.

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Prof. Vivek Polshettiwar research interests are within the domain of advanced nanomaterials and nanocatalysis for harvesting solar energy and the transformation of carbon dioxide into value-added chemicals and fuels. The work of his group in the nanocatalysis realms of "Black Gold" and "Defects" chemistry represents a quintessential example of how fundamental science can drive innovation in applied research. He is the recipient of the prestigious ORISE Research Fellowship at US-EPA. He also received an Asian Rising Star lectureship at 15th Asian Chemical Congress (ACC), Singapore (2013), from Nobel Laureate Professor Ei-ichi Negishi. In 2015, he was admitted as a Fellow of the Royal Society of Chemistry (RSC), United Kingdom. He was awarded a Bronze medal by the Chemical Research Society of India (CRSI), India. He was awarded the prestigious Materials Research Society of India - MRSI Medal 2019. In 2021, he was elected as a Fellow National Academy of Sciences, India (NASI). He received the 2022 IUPAC-CHEMRAWN VII prize for green chemistry from IUPAC. In 2023, he received the Falling Walls Award in Physical Sciences. In 2024, he was elected as a Fellow Indian Academy of Sciences. In 2024, he was Awarded Prestigious Vigyan Yuva-Shanti Swarup Bhatnagar (VY-SSB) Award by the President of India.

KN-26: Role of CCS in India's Efforts in Decarbonization

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Abstract

India stands on the brink of a significant economic transformation, poised for rapid development. This growth is expected to drive increased energy consumption, predominantly from coal and petroleum. Ambitious targets across various sectors—especially in "hard-to-abate" industries like power, steel, cement, petroleum, and fertilizers—will contribute substantial anthropogenic CO₂ emissions. Modeling projections suggest that meeting the net zero target would likely require substantial amounts of CO₂ capture and storage. Our recent estimates on CO₂ storage potential in Indian geologic formations through different pathways: enhanced oil and gas recovery (EOR), enhanced coal bed methane recovery (ECBMR), deep saline aquifers, and basalts indicate sufficient storage capacity to store the captured CO₂. Depleting oil fields and unminable coal seams should be actively considered within policy-making as they predominantly lie within areas of dense areas of large point sources (LPS), thus creating possibilities of CCS hubs and clusters. Moreover, a number of saline aquifers are characterized as having storage potential equivalent to several years of LPS emissions along with high storage feasibility. Preliminary source-sink mapping results show substantial clustering opportunities in eastern India, which has active coalbed methane extraction, and western India, with large industrial sources interspersed with EOR sites.

By achieving five of the UN's seventeen Sustainable Development Goals through CCUS, India can join the league of major world economies on the CCUS world map. As per the International Energy Agency and the Global CCS Institute assessments, CCUS shall account for about 14-32% of all efforts to clean energy transitions by 2070. This work discusses the early opportunities for CCUS in India, its relevance to net-zero emission goals and the scale of carbon sequestration in different geological sinks in the country (1-3).

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Prof. Vikram Vishal serves as a Professor in the Department of Earth Sciences and Centre for Climate Studies at IIT Bombay, and holds a PhD degree jointly from IIT Bombay and Monash University, Australia. His academic and professional journey includes roles at MIT, USA, IIT Bhubaneswar, IIT Roorkee, Tata Steel and Shell. He also implemented his post-doctoral research at Stanford University. Since 2017, Prof. Vishal has served as a faculty member at the US-Department of Energy sponsored 'Research Experience in Carbon Sequestration' school. He is the Convener of the DST-National Centre of Excellence in CCUS at IIT Bombay and is also the founder and director of UrjanovaC Private Limited - a multiple-award winning clean energy and net zero solutions company. An expert on CCUS science, technology and policies, he is a lead investigator for several R&D projects and also serves on several national and international expert committees. Prof. Vishal is a three-time national award and two-time Fulbright fellowship recipient, has authored over a hundred research publications and received five patents. He has co-authored several roadmaps/atlas by the Govt. of India apart from a few international reports.

KN-27: Plastic circularity: Grand Challenges in Chemical Recycling and a New Class of Polyolefins Molecularly Designed for Circularity

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Abstract

The world has cumulatively produced more than 8 billion MT of plastics since 1950 and only 9% of it has ever been recycled¹. This situation is unsustainable. Recycling of plastics faces several complex challenges – availability at scale and heterogeneity of plastic feedstocks, high capital intensity of recycling units and technoeconomic challenges associated with the scale-up². Plastics are recycled using two basic processes – mechanical recycling and chemical recycling. Mechanical recycling is cost-effective but is hampered by the lack of availability of high-quality clean feedstocks and results in a product with inferior properties that can only be used in low-value applications. Chemical recycling involves conversion of mixed plastic waste into pyrolysis oil that can be blended with refinery products such as naphtha and thermally cracked to produce olefins that are polymerized to produce virgin plastics. In the first part of my talk, I will focus on the grand technoeconomic challenges in scaling up chemical recycling of plastics. These technoeconomic challenges are rooted in the complexity of the feedstocks that necessitates multi-step decontamination of the intermediate products and transport limitations that result in high capital intensity. In the second part of my talk, I will describe a novel class of polyesterolefins that demonstrate material properties similar to polyolefins but are molecularly designed for ease of chemical recycling through well-known and scalable chemical routes³.

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Leader, Polymer and Material Science Department, Corporate R&D, directly responsible for five large global teams in Europe, USA and KSA (Kingdom of Saudi Arabia) adding to 80 scientists and engineers who are working to build innovation program portfolio (NPV >\$1 billion) focused on development of novel materials to support energy transition and development of “design for recycle” polymers to support circular economy. Previously led Engineering Science department that was focused on developing a suite of technologies to convert cost-advantaged feedstocks to olefins and other petrochemicals and next generation technologies for plastic-to-plastic value chain in circular economy. Experience with successfully leading large cross-functional global teams to spearhead process/product innovation from ideation through piloting and scale-up to manufacturing plants for technology commercialization. A systems thinker with a customer-centric approach towards process/product development and a successful track record to drive organizational change. Expert in new process/product development, scale-up to manufacturing and technology commercialization in chemical plants, R&D program portfolio management, technology portfolio for circular economy, certified lean six sigma black belt, pilot plant management, design and optimization of chemical processes

KN-28: New Avenues in Radical Based Approaches to Heterocycles

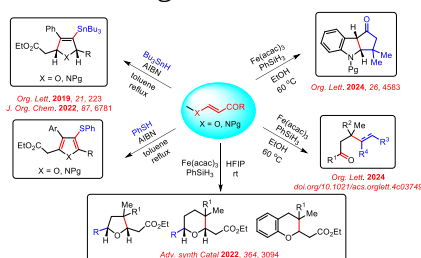
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Abstract

Heterocycles such as substituted tetrahydrofurans (THFs), tetrahydropyrans (THPs), chromans, and pyrroles are important scaffolds in many natural products and biologically active compounds. Although, vinylogous carbonates/carbamates have emerged as excellent radical acceptors for the synthesis of cyclic ethers, their utility for the synthesis of furan/pyrrole derivatives remains underexplored. In this context, we have reported the divergent synthesis of tetrasubstituted furans, dihydrofurans and pyrroles using $\text{Bu}_3\text{SnH}/\text{PhSH}$ mediated cascade radical cyclization on vinylogous carbonates and carbamates. In recent years, metal hydride hydrogen atom transfer (MHAT) radical hydrofunctionalization of isolated olefins has emerged as a powerful tool for the construction of carbon–carbon and carbon–heteroatom bonds. We have showcased utility of MHAT for the synthesis of heterocycles such as THFs, THPs, chromans as well as fused indoles/pyrroles. The talk will focus on these studies and interesting new discoveries made along the way.



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Dr. Santosh J. Gharpure graduated with an M.Sc. degree in 1996, from Indian Institute of Technology Bombay, Powai. He obtained Ph.D. from Indian Institute of Science, Bangalore working with Late Prof. A. Srikrishna in 2001. He held a post-doctoral position with Prof. P. Andrew Evans at Indiana University, Bloomington, U.S.A. Subsequently, he joined the Department of Chemistry, IIT Madras, Chennai in the year 2004. In 2012, he moved to the Department of Chemistry, IIT Bombay, Powai, Mumbai as an Associate Professor and was promoted to Professor position in 2016. Currently, he holds the position of ‘Rasiklal Hemani Fragrance and Flavour Chair Professor’. He is also Professor In-Charge of SINE, IIT Bombay’s technology incubator. His research focuses on organic chemistry pertaining to natural and unnatural product synthesis and developing new synthetic methodologies. He is also working on problems relevant to industries from different domains. Dr. Gharpure is a recipient of INSA Medal for Young Scientist. He was awarded IIT Madras Young Faculty Recognition Award (YFRA) for his contribution in teaching and research in 2010. He received B. M. Birla science Prize in Chemistry for the year 2011. He was selected as one of the Thieme Chemistry Journal Awardees for the year 2013. IIT Bombay conferred on him the Excellence in Teaching Award in the year 2015 and Departmental award for excellence in teaching in 2019. He was selected as Themis Medicare UICT Diamond Jubilee Distinguished Fellow in Pharmaceutical Science for the year 2015-16 of ICT, Mumbai. He was selected for the award of Chemical Research Society of India (CRSI) Bronze Medal in 2018. He is member of the International Advisory Board of European Journal of Organic Chemistry, Tetrahedron and Tetrahedron Letters. He is a Fellow of Royal Society of Chemistry (FRSC). He was awarded INSA Teachers Award 2021 by Indian National Science Academy, New Delhi.

Invited Speakers

IL-1: Ligand-Directed Ammonia Synthesis Using Visible Light and Quantum Dots

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Abstract

The large absorption cross-section and high photostability of plasmonic nanoparticles (NPs) and quantum dots (QDs) make them ideal candidates for various solar-to-chemical fuel conversions.^{1,2} However, achieving an efficient separation and utilization of charge carriers from NPs/QDs is still challenging.^{2,3} Our group has developed strategies based on the interplay of forces, via appropriate ligand chemistry, to improve the charge separation and utilization steps in NP/QD photocatalysis.⁴ By introducing the idea of favourable catalyst-reactant interactions, we were not only able to achieve efficient photocatalysis at low catalyst concentration, but also regulate the catalytic properties between completely 'ON' and 'OFF' states - rendering the same NP as a catalyst or a non-catalyst as per the demand.⁵⁻⁹ In this presentation, I will be showcasing the power of surface ligands on InP QDs in photocatalysing the synthesis of ammonia from nitrate and nitrite ions.¹⁰ The presence of catalytic indium sites and microenvironment modulation through an interplay of catalyst-reactant interactions resulted in efficient and selective ammonia formation under visible light. In summary, the use of electrostatics mimic the underlying force involved in various enzyme catalysis, which can serve as a generic approach for other important multielectron photocatalytic reactions.

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Prof. Pramod Pillai is an Associate Professor in the Department of Chemistry at Indian Institute of Science Education and Research (IISER) Pune, India. Prof. Pillai obtained his Ph.D. in 2008 under the supervision of Prof. K. George Thomas at the National Institute for Interdisciplinary Science and Technology (NIIST) Trivandrum, India. Prior to joining IISER Pune in June 2014, Prof. Pillai was a postdoctoral fellow in the group of Prof. Bartosz A. Grzybowski at Northwestern University, Evanston, USA (2011-2014), and an Alexander von Humboldt postdoctoral Fellow at Technische Universität in Dortmund, Germany with Prof. Christof M. Niemeyer (2008-2010). Currently, Prof. Pillai's research at IISER Pune is focused on controlling the interplay of forces to improve and impart newer properties at the nanoscale. Some of the properties of interest include artificial photosynthesis, plasmonics, and self-assembly. Prof. Pillai is in the Editorial Board of *ChemNanoMat*, a journal published by the Wiley Publishing Group.

IL-3: Intermolecular Interactions and Dielectric Screening Effects on Core-Level Shifts, and X-Ray Emission Spectroscopy

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Abstract

Recent and continual advancements in the areas of X-ray spectroscopy have enabled the investigation of core-level spectroscopy of high vapor-pressure liquids such as water and ammonia. However, an atomistic understanding of core-level shift of liquids compared its gas-phase analogues is an emerging and frontier challenge. In this talk, I will discuss how the development of a hierarchy of electronic structure methods can aid in the modeling of such core-level shifts. I will quantify the importance of intermolecular electrostatics and screening effects in determining the core-level shifts in liquids. Finally, I will present core-hole free electronic structure methods to model non-resonant X-ray emission in molecular systems.

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Dr. Vamsee is the head of the Quantum Chemistry group at TIFR, focusing on developing theoretical frameworks and computational tools for understanding one-electron properties. He actively contributes to the development of the TURBOMOLE software. His research spans response theory-based method development, efficient computation of one-electron properties, and studying intermolecular interactions. His additional interests include fluctuating-charge force fields, charge-transfer pathways in confined systems, and the mechanisms of plasmon-mediated catalytic processes.

IL-3: Efficient Economical Energy Harvesting from Plastic and Electronic Wastes Using Human Bodily Motions

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Abstract

Waste management of plastic and electronic artefacts is a very tedious task and requires a great deal of expense. The pressing threat to the environment due to excessive plastic use and uncategorized electronic waste management demands versatile strategies to mitigate the said issues.¹ Therefore, my talk addresses a very simple and affordable method for creating a triboelectric nanogenerator (TENG) out of plastic and electronic waste. Triboelectric layers were made using recovered polyethylene terephthalate (PET) from used Kapton tape and printing paper². More crucially, a straightforward copper sacrificial electrodeposition method was used to create the electrode layers instead of complex and extensive procedures. It is an excellent approach to recycle discarded plastics and create gadgets that collect and generate energy from them³. The copper was taken from discarded electrical lines from malfunctioning UPS batteries.

The fabricated TENG delivered excellent electric output with a maximum open circuit voltage of ~552 V, a short circuit current of 18.8 μ A and a high-power density of 7.68 W m⁻² under contact-separation triggered by human hand tapping. A vast number of practical demonstrations include the successful lighting of the 472 LEDs connected in series, storing the charges in commercial capacitors, and powering the digital calculator.

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Thara's research interests include design and development of new materials with focus on energy conversion/storage, in-depth fundamental analysis by various electrochemical, spectroscopic, microscopic and scanning probe techniques.

She is a recipient of several prestigious fellowships like Alexander von Humboldt Postdoctoral Fellowship, Germany and Ramanujan Fellowship by DST. She is a Fellow of Royal Society of Chemistry admitted through "Leaders in the field" scheme and also an elected Fellow of Indian Chemical Society. She is a recipient of CRSI-Bronze Medal 2023 and Silver Medal of CRS 2023 from the Society Chirantan Rasayan Sanstha, ECSI National Metrohm Award 2023 from Electrochemical Society of India and A.V. Rama Rao prize for women 2024 from Chemical Research Society of India. She is an Associate Editor of Chemistry of Materials (ACS), an Editorial Board Member of Electrocatalysis (Springer Nature) and Sustainable Energy and Fuels (Royal Society of Chemistry).

IL-4: Machine Learning for CO₂ Reduction Reactions

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Abstract

Recent research aims to enhance catalysts for the carbon dioxide reduction reaction (CO₂RR), enabling the production of carbon-neutral fuels in an eco-friendly manner. Both experimental and computational methods are being leveraged to improve catalyst activity and selectivity. Machine learning (ML) and data science are essential in speeding up the identification of effective catalysts. In our prior work, we utilized distinctive surface microstructural features within ML models to discover high-entropy alloy-based catalysts for converting CO₂ into methanol.¹⁻⁵

Building on that foundation, we now introduce a novel strategy called Conformal Active Learning (CAL) to assess ligand-protected Cu-nanoclusters for CO₂RR. Both the core metals and the ligands play crucial roles in influencing product selectivity. Our ML model incorporates a comprehensive uncertainty assessment, delivering accurate predictions of catalyst performance while significantly minimizing prediction errors and uncertainties across various datasets. By examining feature importance, we can identify the most critical catalyst descriptors. This allows us to refine the selection criteria based on our predictions, facilitating the efficient screening of catalysts that promote C1 product formation.

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Dr. Biswarup Pathak is a Professor in the Department of Chemistry at IIT Indore, India, where he leads the Computational Materials Designing Research Group. He mentors research scholars in advanced computational modeling using machine learning and artificial intelligence to study nanomaterials, particularly nanoclusters, for applications in catalysis, energy, and biology, including DNA sequencing. Dr. Pathak has published over 275 papers and has more than 7,500 citations (Google Scholar; H-index: 46).

In 2017, he received the Early and Mid-Career Research Award from the Indian National Science Academy (INSA) and collaborated with Prof. Peter Gill at the Australian National University. He has been honoured with the IIT Indore Best Researcher Award in 2016, 2023, 2024 and has secured grants exceeding 4.8 crores from various national and international agencies for his research on nanomaterials.

Dr. Pathak has delivered over 70 invited talks and was featured on the cover of the *Journal of Physical Chemistry's* Young Scientist Issue. Recognized by the American Chemical Society as one of India's most impactful researchers in 2021, he was recently admitted as a Fellow of the Royal Society of Chemistry (FRSC) in the UK and received the CRSI Bronze Medal and MRSI Medal in 2023 for his significant contributions to the field of chemistry.

IL-5: Mitigating the Poisoning Effect of Formate During CO₂ Hydrogenation Using Cobalt Containing Dual-Atom Oxide Catalysts

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Abstract

The hydrogenation of CO₂ to methanol faces challenges due to the competitive reverse water-gas shift (RWGS) reaction, which reduces methanol selectivity. This competition arises from formate intermediates, which can either convert to methanol or CO. Oxide catalysts such as In₂O₃ and mixed oxides can strongly adsorb CO₂ and intermediate species, but this can also hinder hydrogen dissociation, lowering the methanol selectivity.

To address this, a Co-In-ZrO₂ dual-atom catalyst was developed to separate the sites for adsorption and H₂ dissociation. The oxygen vacant site created by Co atom facilitates CO₂ adsorption and formate stabilization, while In atoms dissociate H₂, preventing the poisoning effect and promoting methanol formation. The dual-atom catalyst demonstrated high methanol selectivity (87% at 270°C) and lower activation energy (80 kJ mol⁻¹) compared to single-doped catalysts. Kinetic analysis revealed improved H₂ utilization, further enhancing methanol selectivity.

Contrary to the current approach of increasing H₂ dissociation over oxide catalyst by using noble metals, we show a new strategy of separating sites for CO₂ adsorption and H₂ dissociation to effectively increase both methanol selectivity and yield. This approach allows higher methanol selectivity at low H₂ partial pressure, which is essential to reduce the use of highly valuable renewable H₂ stream.

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Abhijit Shrotri is an Assistant Professor at the Institute for Catalysis in Hokkaido University, Japan. Prior to that he worked as a postdoctoral fellow at the Catalysis Research Center in Hokkaido University (2014 to 2016). He received his Ph.D. in Chemical Engineering from the University of Queensland in Australia (2014). His research interest includes development of heterogeneous catalyst for utilization of CO₂ and biomass derived resources. In particular, he is studying the use of metal oxide catalysts with oxygen vacancy for conversion of CO₂ and development of catalytic processes for synthesis of valuable chemicals from biomass. He was awarded the Encouragement Award from the Catalysis Society of Japan in 2023. He is the recipient of 10th New Chemical Technology Research Encouragement Award from Japan Association for Chemical Innovation, in 2022.

IL-6: Edge States in Low-Dimensional Halide Perovskites: Sites of Efficient Exciton Dissociation

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Abstract

In the realm of perovskite optoelectronics, understanding how excitons behave at the crystal edges is key to unlocking high-performance photovoltaics. Quasi-two-dimensional (2D) layered halide perovskites harbor the unique properties of enhanced exciton dissociation at crystal edges, known as localized edge states. These crystal edges, along with grain boundaries and free surfaces, serve as sites where excitons, bound pairs of electrons, and holes dissociate into free carriers enhanced by the thermal disorder and dangling octahedra bonds present at these locations. Photogenerated excitons from the bulk diffuse to these localized edge states, which are then dissociated into longer-lived free carriers, improving the conductivity of these sites. This high population of free carriers is then extracted by the respective transport layer and collected at the respective electrodes, improving the power conversion efficiency. By carefully controlling the population of edge states at the interface between the perovskite and transport layer, we can significantly boost the power conversion efficiency of quasi-2D layered halide perovskites, bringing us closer to more stable, high-performance photovoltaic devices.

As Nobel Laureate Herbert Kroemer famously said, "The Interface is the Device." This holds true in the realm of perovskite optoelectronics, where the behavior at interfaces can make all the difference in device performance.

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Dr. Sachin Rondiya, currently serving as an Assistant Professor in the Department of Materials Engineering at the Indian Institute of Science (IISc), Bangalore, is at the forefront of interdisciplinary research encompassing physics, chemistry, materials science, and engineering. Dr. Rondiya's primary focus is on developing innovative solutions for energy harvesting, storage, and conservation, with a special emphasis on improving the performance of novel semiconductor materials for solar cells. His research delves deeply into the optical and electronic properties of nanoscale systems, aiming to extend the current knowledge in the solar cell field through fundamental investigations.

IL-7: Biomimetic Studies on the Detoxification of Highly Neurotoxin Organomercurials

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Abstract

Organomercurials (RHg^+), especially methylmercury (Me-Hg^+), are extremely neurotoxic and ubiquitous environmental pollutant, which accumulates at high levels in food chains, mainly in fish and seafood, and therefore, consumption of contaminated foods poses a significant risk to human health. Exposure to ethylmercury (Et-Hg^+) is a serious concern in developing countries where Et-Hg^+ -containing antimicrobial agent “Thimerosal” is commonly used as a preservative in multiuse vials of vaccines and other medicines.

In nature, however, several microorganisms have been reported to detoxify organomercurials including MeHg^+ by converting them to less toxic biologically inert species. For instance, bacterial organomercurial lyase (MerB) catalyzes the protolytic cleavage of the otherwise inert Hg-C bond of MeHg^+ and produces methane (CH_4) gas and ionic mercury Hg^{2+} , while a second enzyme mercuric ion reductase (MerA) reduces the product Hg^{2+} to volatile Hg^0 . On the other hand, several sulfate reducing bacteria (SRB) convert highly toxic MeHg^+ to less toxic insoluble HgS(s) (metacinnabar) by producing H_2S during metabolism. MeHg^+ and EtHg^+ are considered to be more neurotoxic than the inorganic counterpart (Hg^{2+}). They cause massive DNA damage in cells, especially in neurons, where cellular glutathione (GSH) levels are significantly low. However, the mechanism by which RHg^+ exerts massive DNA damage at cytotoxic concentrations in brain cells remains obscure. This talk will focus on the detoxification pathways of mercury-related compounds in the cellular system and also provide a new mechanistic insight into the mode of action of organomercurials in GSH-depleted cells and their adverse effects on individuals with neurodegenerative disorders associated with oxidative stress.

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Prof. Gouriprasanna Roy's research group mainly focuses on two major areas, chemistry, and biology, at the interface of chemistry and biology to understand the homeostasis of essential elements and the detoxification of toxic elements in our body. Our laboratory is involved in the chemical detoxification of various toxic heavy metals such as mercury, arsenic, and copper. Organomercurials are highly neurotoxic environmental pollutants that preferentially accumulate in the glia of the central nervous system (CNS). We aim to understand how methylmercury and ethylmercury, an extremely neurotoxic organomercurial, exerts its neurotoxicity and try to understand the detoxification pathways in the biological system. On the other hand, copper ion is essential in our lives and used as a cofactor in several vital processes. However, high concentrations of copper can be harmful as they promote Fenton-like reactions, thereby increasing the cellular ROS levels and leading to the oxidative damage of cellular constituents like proteins, lipids, and nucleic acids. It is essential to control copper concentration strictly in the body. Prof. Roy was recognized as one of the *Emerging Investigators* in 2019 by *Metallomics*, a leading journal by Oxford University Press. He was awarded a Bronze medal in 2020 by the Chemical Research Society of India (CRSI), India.

IL-8: From Earth to Mars: Pioneering Metal-Carbon Dioxide (Metal-CO₂) Battery Solutions for a Greener Tomorrow

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Abstract

As climate change intensifies, energy solutions for Earth have become crucial towards a sustainable future. Metal-carbon dioxide (CO₂) batteries offer a transformative approach, converting CO₂ into usable energy while addressing carbon management and reducing emissions. Beyond Earth, these batteries hold significant potential for Mars, where CO₂ is abundant (95 %) providing essential power for future colonies, supporting habitats and life support systems. By harnessing the in-situ resources of Mars, metal-CO₂ batteries could enable sustainable living on the Red Planet. However, its practical implementation faces challenges, including low cyclability, high overpotentials, and poor reversibility due to the thermodynamic stability of discharge products like Li₂CO₃ and amorphous carbon.^[1–4]

Our work addresses these challenges by developing unique catalysts including carbon, transition metals, composite nanoparticles. These catalysts enhance the CO₂ reduction and therefore the cyclability of the system. Their bifunctional catalytic behavior helps reduce the activation energy required for the decomposition of the Li₂CO₃ and amorphous carbon, resulting in enhanced reversibility. Benefitting from this, we were able to achieve a cycle life of ~200 cycles at the current density of 500 mA g⁻¹ for a limited capacity of 500 mAh g⁻¹ along with an operational time exceeding 600 hours. Additionally, we explored translating the system from lithium to the more abundant sodium and potassium metals, paving the way for future sustainable energy solutions.^[5–9]

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Chandra Shekhar Sharma is a Professor in the Department of Chemical Engineering at IIT Hyderabad, renowned for his pioneering work in nanomaterials that bridge creativity, innovation, and advanced research to tackle pressing global challenges. His research group specializes in developing functional materials with diverse applications, from pollution mitigation to feminine hygiene and sustainable futuristic energy solutions. With over 150 scientific publications and four granted patents (and 16 patents filed), Prof. Sharma's contributions to the field are both impactful and extensive. In recognition of his excellence, he received several honors including prestigious DST Swarnajayanti Fellowship in 2020 for Engineering Sciences. A leader in fostering scientific engagement, he has chaired INYAS, a prominent academy for young scientists, and in 2024, he was honored to serve as Chair of the Global Young Academy (GYA), promoting scientific innovation among emerging talents. Prof. Sharma's insights and expertise make him an inspiring researcher dedicated to shaping the future of science and technology for a better world.

IL-9: Microscopic Understanding of Dynamic Catalysis Using a Discrete-State Stochastic Approach

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Abstract

Nanocatalysts exhibit spatial heterogeneity, displaying varying catalytic activities across different regions. To study the heterogeneous nature of these nanoparticles, we analyze their stochastic fluctuations, identifying several sources of heterogeneity. In addition to spatial heterogeneity, nanocatalysts can exhibit a dynamic nature, referred to as dynamic catalysis. This dynamic behavior further contributes to the complexity of their catalytic activities. Dynamic catalysis, a phenomenon where the catalytic properties of a system change over time, stands in stark contrast to static catalysis, where the catalytic activity remains constant. This exciting concept has gained attention as a potential alternative to traditional static catalysis, because of potential significant improvements in catalytic efficiency.¹ The microscopic mechanisms of the underlying processes are poorly understood, posing a challenge to researchers aiming to exploit and control these phenomena for improved catalytic performance. We have developed a new stochastic framework that enables the quantitative description of dynamic catalysis, facilitating a comparison of its properties with those of the static approach.^{2,3} Observations indicate that fluctuations between distinct catalytic pathways may enhance chemical reaction rates, albeit within specific ranges of kinetic parameters. We show that the temporal efficiency of dynamic catalysis depends only on the rates of chemical reactions and transitions between different catalytic pathways while being independent of the number of active sites. Dynamic catalysts operate outside of equilibrium conditions, and the energy dissipation associated with this dynamic behavior is the source of improvements in catalytic efficiency.⁴ The stochastic aspects of dynamic catalysis have also been investigated. Our theoretical method can explain these observations from the microscopic point of view and may help build better catalysts.

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IL-10: Can Visible Light Do Selective Dearomative C-H Activation

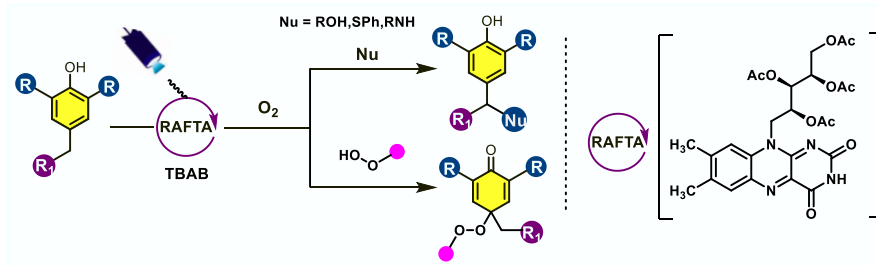
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Abstract

Aromatic hydrocarbons are the economic class of feedstock which are available in plenty all around. Generation of multi-functional three-dimensional structures from these simple planner aromatic compounds allow a fast access to solve complexity at higher levels. The focal point lies on the fact, that a wide range of carbon-carbon and carbon-heteroatom bond formations are possible with this key transformation. Specially, the CADR's developed by You. *et. al.* has attracted a world-wide attention. Transition metal complexes based on Os, Ru, Re, Cr, Mn etc. in stoichiometric amounts have shown predominance in these transformations, the toxicity and cost related to the use of these complexes behave as deterrents of their ample use in synthesis. The exhaustive resonance stabilization renders arenes particularly unreactive as starting materials. Protocols which can circumvent this inertness are scanty. This inertness often leads to side reactions like dimerization and decomposition of the substrate. Notable contribution from our lab includes the tribromides as key resource of dearomatization. Our perruthenate generated catalyzed *ipso*-dearomative spiro-etherification and spiro-amidation of phenols delivers an insight catalytic dearomative spirocyclisation. Albeit, we envisioned that a photocatalytic oxidation of phenols with visible light in presence of aerial oxygen as oxidant would be a certain advancement of dearomative chemistry.



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IL-11: Asymmetric C-H Bond Functionalizations Under Cobalt Catalysis

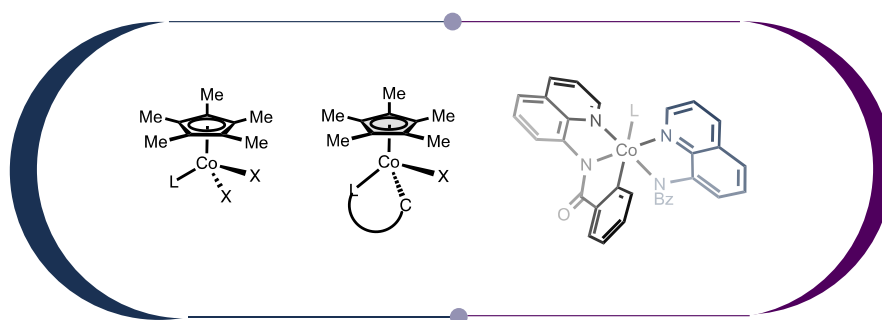
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Abstract

Since Murahashi's pioneering work on cobalt-catalyzed C-H bond carbonylation in 1955,¹ the field of C-H bond functionalization has evolved significantly, particularly with the advent of low-valent cobalt systems.² While the use of in situ-generated or isolated cobalt(III) catalysts for C-H activation was rarely explored until Daugulis's 2014 report, recent advancements have shed light on the intricate coordination environment surrounding cobalt and the mechanisms involved in these catalytic cycles. In this talk, I will delve into the role of external chiral ligands and the induction of chirality at the metal center through a rate-limiting C-H activation step, illustrating how these factors influence the efficiency and selectivity of asymmetric transformations.⁴ Additionally, I will present innovative strategies employing photocatalysts^{5a} or oxygen^{5b} as sole oxidants, which effectively eliminate the need for stoichiometric metal oxidants in our asymmetric C-H bond annulations using the Co/Salox catalytic system. This discussion will highlight both the fundamental insights gained and the practical applications arising from this evolving area of research.



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Dr. Basker Sundararaju is an accomplished researcher in the field of catalysis, specializing in developing innovative and sustainable catalytic methods to transform chemical reactions. With a strong focus on transition metals and organometallic chemistry, their work aims to design efficient catalytic systems for regio-, stereo-, and enantioselective reactions, minimizing hazardous waste and advancing green chemistry. Their research integrates ligand design, mechanism elucidation, and targeted molecular synthesis to contribute to environmentally sustainable processes. Dr. Basker Sundararaju has received notable accolades, including the Thieme Chemistry Journal Award (2014), the DAE-BRNS Young Scientist Award (2014), and the Alexander von Humboldt Fellowship (2012–13).

IL-12: Tailored Molecular Diffusion in Nanoporous Material for Separation and Catalysis

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Abstract

Chemical separation and catalysis are vital industrial processes, with porous materials playing a central role in these applications. Over the past two decades, significant attention has been given to exploring the potential of crystalline porous materials, such as metal-organic frameworks (MOFs) and covalent organic frameworks (COFs), due to their unique structural and chemical properties. Among the critical factors influencing their performance is molecular diffusion, which directly impacts the efficiency of chemical separations, turnover frequencies, and selectivity in catalytic reactions.

In my talk, I will provide an overview of our research focused on fine-tuning molecular diffusion within nanoporous MOFs.¹⁻⁴ I will highlight a recently developed methodology for controlling chemical diffusion, which enables the achievement of maximum catalytic efficiency.⁵ This includes optimizing turnover frequency and geometric selectivity, demonstrated using a MOF catalyst for a condensation-type organic reaction.

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Ritesh Haldar earned his PhD from JNCASR (2015), Bangalore under the supervision of Prof. Tapas Kumar Maji. Before joining TIFR Hyderabad as Reader F, Ritesh was Alexander von Humboldt postdoctoral fellow and junior group leader at Karlsruhe Institute of Technology. Since 2021, Ritesh has established a research group at TIFR Hyderabad focusing on understanding of chemical diffusion process in nanoporous materials and their application in chemical separation and catalysis. His research group develops gas and liquid chemical separating membranes, methodology for hybrid heterostructure thin films and flow heterogeneous catalysis.

IL-13: Low-temperature Catalytic Hydrogen Production Reactions

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Abstract

Hydrogen is a clean energy source, and when used in fuel cell produces only water as a by-product.¹⁻⁵ However, carrying big and heavy hydrogen cylinders with high pressure has critical safety and economical challenges. Alternatively, using liquid hydrogen storage material in the fuel tank of existing vehicles (using petroleum products) and generating hydrogen on-board to supply to fuel cell is not only a viable concept but is also very economical. In this context, worldwide scientific efforts are concentrated on the hydrogen carriers such as methanol, ethanol and polyols, which are not only stable, safe to handle and transport but also release hydrogen under relatively mild conditions in the presence of a suitable catalyst.¹⁻⁵ Despite that reforming of these alcohols/polyols yield H₂ gas but it also releases equivalent/more CO₂.

In this work, we developed processes where only purified H₂ gas is produced from these alcohols/polyols, while all carbon content is transformed into value-added products. For instance, methanol releases 2 equiv. of H₂ along with formate.^{1,2} On the other hand, glycerol yields 1 equiv. of H₂ along with 1 equiv. of lactic acid.⁵ We demonstrated the critical role of catalysts in tuning the dehydrogenation pathway.

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Prof. Sanjay K. Singh's research interest is focused on the development of catalysts and catalytic processes for hydrogen production, biomass/waste transformation and carbon dioxide capture and conversion to value-added products and fuel components. He is the recipient of the prestigious Alexander von Humboldt Fellowship for research stay at KIT Germany (2024). He also received S.S. Deshpande Award (2022) and Bronze Medal award by the Society of Materials Chemistry, India (2024). He is also Editorial Board member of ChemCatChem (since 2022) and Editorial Advisory board member of ACS Sustainable Chemistry and Engineering (since 2023).

IL-14: A Multiscale Understanding of how Oscillating Bubbles Orchestrate Chemistry in Sonochemical Reactors

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Abstract

Non-thermal approaches to driving chemical reactions using light, ultrasound, plasma, mechanical forces, and microwaves, are having a renaissance with the inevitable electrification of the chemical industry. Ultrasound irradiation is particularly interesting, given its ability to generate free radicals (oxidants) under nominally ambient conditions of 300 K and 1 atm. pressure. Such oxidants enable chemistries that otherwise do not occur under ambient conditions. Ultrasound irradiation is already used in the industry for mixing, cleaning materials, and wastewater treatment. Recent studies have shown the promise of ultrasound irradiation for specialty chemical synthesis. For example, ultrasound irradiation depolymerizes cellulose to glucose, and selectively oxidizes glucose to high-value acids. Notwithstanding the decades of progress in ultrasound mediated chemical reactions, we do not yet possess a molecular-level understanding of how free radicals, generated in situ by cavitating bubbles, orchestrate selective chemistries in sonochemical reactors. Establishing this molecular level understanding is vital towards designing more energy efficient sonochemical reactors. To address this knowledge gap, we present a multiscale framework to advance the foundational knowledge of how ultrasound mediated reactions occur. This framework unites quantum chemistry calculations at the nanometer scale, heat/mass/momentum transport models for cavitating bubbles at the micrometer scale and mean-field kinetics of reaction networks in batch reactors at the meter scale. This multiscale framework is calibrated with experiments and is applied to the oxidation of benzyl alcohol and glyoxal. Using this framework, we not only elucidate how and why reactions occurring in sonochemical reactors can be selective, but also demonstrate how this mechanistic understanding will lead to more energy efficient sonochemical reactors.

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Tej graduated with a B. Chem. Engg. from the Institute of Chemical Technology (formerly known as UDCT) in 2012. He obtained his PhD in chemical engineering from Purdue University in Dec. 2017 under the supervision of Prof. Jeffrey Greeley. He thereafter completed his postdoctoral training at the SUNCAT Center for Interface Science and Catalysis at Stanford University under the supervision of Dr. Frank Abild-Pedersen in Nov. 2019. Tej joined NTU in Dec. 2019. His group employs first principles methods and kinetic modelling to understand how catalysts operate at the atomic scale. These atomistic insights are thereafter used to design improved catalysts. Tej has over 34 peer reviewed journal publications and his research program has attracted funding from both governmental and industrial sources. Tej has received several awards including being an Early Career Distinguished Presenter at the Materials Research Society Meeting (2024), Young Talent Laureate from the International Catalysis Congress (2024), Emerging Investigator of Reaction Chemistry and Engineering (2022), and the Outstanding Young Principal Investigator of the AIChE, Singapore Local Section (2022). Tej holds early career leadership positions in editorial boards of academic journals like *ChemSusChem*, *Journal of Catalysis*, and *Applied Catalysis A: General*. Tej was awarded the Nanyang Education Award (School) for excellence in teaching in 2022.

IL-15: Chemistry of Heterogeneous Catalysis for Sustainable Green Hydrogen Energy

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Abstract

Semiconductor based photochemical and photoelectrochemical water splitting is an ultimate source of hydrogen generation as renewable green energy for tackling the ongoing fuel crisis. Carbon based materials are ideal for overall water splitting as a result of the excellent alignment of its band edges with water redox potentials. However, a single catalyst with a limited number of active sites does not exhibit significant photo/electrocatalytic activity for hydrogen production. Therefore, we have developed the semiconductor heterostructures of carbon materials with oxides, sulphides, selenides, other TMCs/TMDs NPs and QDs as the highly efficient nanocatalysts for enhanced hydrogen evolution reactions. The monophasic heterostructures have been designed in different weight ratios with fairly uniform distribution of nearly spherical particles and high specific surface area which creates an interfacial charge transfer between two semiconductors. As prepared heterostructures showed significant hydrogen evolution which is evident by observing high apparent quantum yield, low onset potential, lower overpotential and high electrochemical active surface area that will be presented in detail.

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Prof. Tokeer Ahmad is graduated from IIT Roorkee and Ph.D. from IIT Delhi. Presently, he is full Professor at Department of Chemistry, Jamia Millia Islamia, New Delhi since 2019. Prof. Ahmad has supervised 16 PhD's, 79 postgraduates, 10 projects, published 205 research papers, one patent and three books with research citation of 8100, h-index of 53 and i10-index of 163. Prof. Ahmad is active reviewer of 186 journals, delivered 180 Invited talks, evaluated 65 external doctoral theses and presented 130 conference papers. Prof. Ahmad is the recipient of CRSI Bronze Medal, MRSI Medal, SMC Bronze Medal, ISCAS Medal, Inspired Teacher's President of India Award, DST-DFG award, Distinguished Scientist Award, Maulana Abul Kalam Azad Excellence Award of Education, Teacher's Excellence Award, Elected Member of National Academy of Sciences India and Fellow of Royal Society of Chemistry (FRSC), UK.

IL-16: The Rise of Single Atom Catalysts: Synthesis and Catalytic Applications

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Abstract

Understanding the relationship between a heterogeneous catalyst's (single atom and nanocatalysts) structure and properties is critical to its progress. The single atom materials are a backbone of many contemporary benign organic transformations and technologies. Over the recent decade, several advanced synthesis approaches have been developed, such as control synthesis of atomically precise single atoms catalysts and their applications for several key applications in organic catalysis/transformations.

Catalyst activity and selectivity have risen exponentially; thanks to the capacity to tailor precise atomic-scale control. Notably, the mechanistic aspects by DFT, EPR study will be discussed. The synthesis, characterization, and applications of single-atom catalysts and nanocatalysts for the organic transformations will be the focus of this lecture.

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Prof. Manoj B. Gawande received his Ph.D. degree in Chemistry in 2008 from the Department of Chemistry, Institute of Chemical Technology, (Formerly UDCT) Matunga, Mumbai, India, under the supervision of Prof. R.V. Jayaram. In 2013, he worked as a Visiting Professor at Division of Chemistry and Biological Chemistry, Nanyang Technological University, Singapore. Presently, he is working as an Associate Professor at Institute of Chemical Technology, Mumbai Marathwada Campus Jalna. During his stay at RCPTM, Palacky University, he has several visiting professor/scientist positions including Prof. Steve Ley (Cambridge University, Cambridge United Kingdom), Prof. Dunwei Wang (Boston College, Boston, Chestnut Hill, MA, USA), and Prof. Rajender S. Varma (EPA, Cincinnati, USA). His research interests are in the development of greener raw materials and synthesis of nano-materials and their applications in sustainable chemistry. He has published more than 170 scientific publications, including reviews, patents, papers, editorial and commentary articles (more than 18,000 citations). Recently he has elected as "Life Fellow" of the Indian Chemical Society. Also, Prof. Gawande has been awarded the prestigious "RSC Research Fund" grant 2021 by the Royal Society of Chemistry (RSC), Cambridge, UK. Dr. Gawande is an editor of several leading journals including Executive Advisory member for by ACS Sustainable Chemistry and Engineering (ACS publications); Current Organic Chemistry (Bentham publications), Associate Editor for Current Catalysis, Regional Editor (Europe zone) for Current Organic Synthesis (Bentham Publications).

IL-17: Harnessing Light to Propel C-H Functionalization

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Abstract

The robust, predictable, chemo- and site-selective conversion of a C-H into a C-X (X = carbon and heteroatom) bond represents the holy grail in organic chemistry.¹ Moreover, direct C-H functionalizations play a pivotal role in developing new chemical entities (NCEs) and drug discovery processes as they enable rapid diversification of pharmaceutical molecules to an exciting range of closely related bioactive analogs and thus allow access to unexplored regions of chemical space. Visible light-induced synthesis provides a sustainable platform to achieve direct C-H functionalizations under mild conditions. Accordingly, our group has developed photoinduced site-selective methods for the direct Csp²-H alkylation of azauracils and other biologically relevant heterocycles,² and Csp³-H alkylation of dihydroquinoxalinones³ using *N*-(acyloxy)phthalimides (NHPI esters)⁴ as alkyl radical surrogates. We have also been successful in demonstrating C-H arylations of several bioactive heterocycles, glycine derivatives, and peptides in a site-selective manner using diaryliodonium reagents (DAIRs) as aryl radical progenitors under visible light irradiation.⁵⁻⁶

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Dr. Murarka's current research activities include the study of novel activation modes and the development of chemoselective and sustainable synthetic transformations. His research group is utilizing sustainable chemical tools, such as base-metal catalysis, photocatalysis, and electroorganic synthesis, to convert feedstock chemicals to value-added compounds and pharmaceutically relevant molecular architectures. He is a recipient of the prestigious 'Institute Senior Researcher Award (Science Category)' by IIT Jodhpur, 'The Early Career Research Award' by SERB, Government of India, 'The Thieme Chemistry Journal Award' by Thieme, and 'The Merck Young Scientist Award' by Merck. He is an Early Career Advisory Board Member (ECAB) of several journals, such as ChemistrySelect (Wiley-VCH), Chemistry an Asian Journal (Wiley-VCH), and Organic Chemistry Frontiers (RSC). He is also a Fellow of the Indian Chemical Society and a Member of the Royal Society of Chemistry.

IL-18: Unleashing the Potential of Novel CO₂ Transformation Technologies

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Abstract

Decarbonization of energy sector is one of the most pressing challenges of the modern era and must be achieved to combat climate change. Accomplishing this goal will require the development of new technologies such as biomass utilization, carbon capture and utilization (CCU), together with revival of existing technologies which enable low-carbon infrastructure. However, the economics of large-scale CCU deployment remains a significant challenge.

This presentation introduces harmonized experimental and modelling approach for optimize and accelerate the deployment of CO₂ capture technologies. We focus on advanced solutions, including novel solvent-based approaches, and innovative calcium looping systems. Our aim is to reduce costs and enhance efficiency through material innovation and integrated process design intensification, making large-scale CCU projects more economically viable, feasible and desirable.¹⁻²

Additionally, we explore the role of AI/ML, deep learning in reactor design, material screening and process scale-up.¹⁻² We further highlight few potential reactions that have not been explored yet but are expected to be viable based on already established methods. Finally, we conclude with a critical discussion on current R&D trends, industrial practices and development of new benchmarking standards which will be quite necessary to accelerate this growing field towards practical application.

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Dr. Komal is currently working as an Assistant Professor in the Department of Chemical Engineering, IIT Roorkee. Prior to this, she was associated as R&D Scientist with UOP Honeywell where she was working in various exploratory areas such as CO₂ Electro-reduction and Green Hydrogen. She earned her Ph.D. from Indian Institute of Technology (IIT) Delhi and M.Tech. from IIT BHU, Varanasi. Her broad research interests include CO₂ reduction, Catalysis, Reaction Engineering and Green Engineering. She is also actively involved in multiple government and industry-funded projects. She has published several research articles in reputed international journals, book chapters and patents. She has received numerous accolades, including the CO₂ INDIA award and the Lovraj Kumar Memorial Trust (LKMT) award for Best Research. She has also won several innovation challenges, been recognized as the Best Auditor for enhancing productivity and cost savings, and been honored for her exceptional skills in incident investigation and preventive action planning in Honeywell.

IL-19: Hybrid Metamaterials with Controllable Twist

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Abstract

Chirality is a geometrical property described by continuous mathematical functions. However, in chemical disciplines chirality is often treated as a binary left/right characteristic of molecules rather than a continuity of chiral shapes. While being theoretically possible, a family of stable chemical structures with the same shape and progressively tunable chirality is yet unknown. Here we present such structures in the form of nanostructured microparticles with anisotropic bowtie shape and widely tunable twist angle, pitch, size, thickness, and length. The self-limited assembly of the bowties made from cadmium and cystine enables high synthetic reproducibility, size monodispersity, and computational predictability of their geometries for different assembly conditions. The bowties nanoassemblies display multiple strong circular dichroism peaks originating from absorptive and scattering phenomena. Unlike classical chiral molecules, these particles display a continuum of chirality measures that correlate exponentially with the spectral positions of the circular dichroism peaks. Bowtie particles with variable polarization rotation were used to print photonically active metasurfaces with spectrally tunable positive/negative polarization signatures for light detection and ranging (LIDAR) devices [1]. Avenues for utilizing the bulk scale synthesis of chiral metamaterials for applications in the field of biosensing [2,3], spintronics, and spectral encryption [4] will be further discussed.

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Prof. Prashant Kumar research interests are within the domain of advanced manufacturing and healthcare materials for precise sensing of biomolecular chirality through optical spectroscopy and analytical transmission electron microscopy. The work of his group in the multiscale synthesis of chiral metamaterials represents a quintessential example of how nanostructure visualization through advanced microscopy techniques can drive innovation in applied research. He is the recipient of the prestigious 35 innovators under 35 in the Asia-Pacific region by MIT Technology Review for the year 2024. He also received the MRS graduate student medal and the MSA presidential scholar award in 2017 for his groundbreaking work on transmission electron microscopy of 2D porous materials. He holds a Bachelor's and Master's in Metallurgical and Materials Engineering from the Indian Institute of Technology (IIT), Madras (2012) and earned his Ph.D. in Materials Science (2018) at the University of Minnesota, Twin Cities, focusing on analytical transmission electron microscopy. His post-doctoral work was performed at University of Michigan, Ann Arbor. Passionate about microscopy, he advocates for STEM careers and mentors aspiring scientists. Beyond research, he finds joy in yoga and weightlifting.

IL-20: Synthesizing Robust Au Cluster Catalysts with Defined Numbers of Au Atoms on Heterogeneous Supports Using Non-Covalent Ligand-Support Interactions

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Abstract

Heterogeneous metal-supported catalysts are indispensable for achieving a sustainable future in terms of their stability and reusability with great catalytic performances. However, constructing well-defined active sites of metal particles on the solid support, such as precise control of constituent atoms or alloy compositions, is still challenging. We have tackled these synthetic challenges by synthesizing atomically precise Au clusters protected by various organic ligands and removing the ligands on the support by thermal treatment since the presence of surface ligands significantly reduces the catalytic activity.¹⁻³ Although this is a promising method to form precise cluster catalysts, there is also a problem with this method: the obtained bare clusters usually have low stability even on the solid supports and easily lose their accuracy which hinders catalytic applications of these materials.

Recently, we have developed a new approach to suppress aggregation using non-covalent ligand-support interaction (Figure 1).^{2,3} Multiple interactions between ligands and supports, such as van der Waals interactions of the organic ligands and carbon support, or electrostatic interactions of carboxylate moiety of the ligand and layered double hydroxide, stabilized atomically precise Au cluster during not only calcination conditions but also catalytic conditions. We revealed the oxidation catalytic properties of these well-defined Au cluster catalysts.

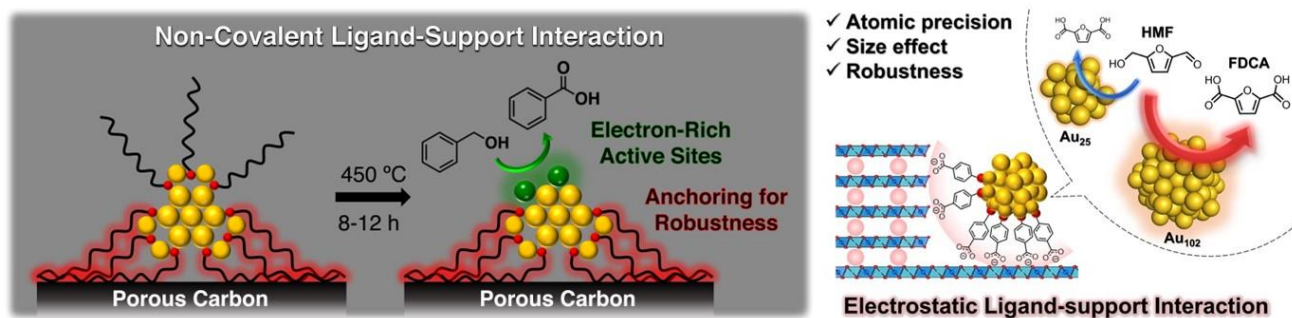


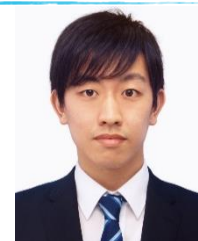
Figure 1. Schematic illustrations of our approaches to constructing atomically precise Au cluster catalysts.

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Specially Appointed Assistant Prof. Shinya Masuda received his Ph.D. in 2020 from Osaka University (Japan) under the supervision of Prof. Hiromi Yamashita. He worked on developing active heterogeneous metal nanoparticle (NP)/cluster-based catalysts for achieving efficient energy conversion catalysis. He became an assistant professor at The University of Tokyo in 2020. His recent research interest lies in revealing the relationship between catalytic performances and physicochemical properties of metal clusters/NPs. To this end, my group has been synthesizing Au cluster catalysts composed of precise numbers of Au atoms on heterogeneous solid supports using ligand-protected Au clusters with atomic precision as precursors. He recently received the Young Researcher Award from Tanaka Kikinzoku Memorial Foundation in 2022.

IL-21: Machine Learning-Assisted Exploration of Materials and Mechanisms for CO₂ Capture and Conversion

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Abstract

Research problems involving the capture and conversion of carbon dioxide (CO₂) form some of the most pressing global challenges, due to the onslaught of climate change. The capture of CO₂ from flue gas and its thermo/electrochemical conversion to valuable chemicals are the key to a sustainable future. Our group combines quantum-mechanical density functional theory (DFT) calculations with molecular dynamics (MD) and kinetic Monte Carlo (KMC) simulations to understand the molecular underpinnings of separations and catalysis using nanomaterials. In this talk, I will present our recent work on the design of nanopores in two-dimensional (2D) materials for CO₂ separation applications, by combining DFT calculations with KMC/MD simulations and machine learning. I will discuss the development of a machine-learnable string representation of nanopores to discover nanoporous graphene structures that can be used to sieve CO₂ from flue gas. I will also present catalyst exploration efforts, wherein we use atomic-scale simulations to unravel new mechanisms for CO₂ reduction to various chemicals on pure/doped copper and 2D materials. I will explain the development of machine learning models to predict activation (free) energies of elementary chemical reactions on a catalyst using various physical features of adsorbate species and chemical transformations. Coupled with automated reaction enumeration and elementary reaction identification strategies, the use of such predictive machine learning models allows the exploration of complex reaction pathways involving thousands of elementary steps. Overall, the multi-scale simulations presented in this talk will help understand and advance the use of nanomaterials for CO₂ capture and conversion processes.

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Dr. Ananth Govind Rajan is an Assistant Professor and Infosys Young Investigator in the Department of Chemical Engineering at the Indian Institute of Science. Dr. Ananth received his B.Tech. from the Indian Institute of Technology Delhi (2013) and his Masters (2015) and Ph.D. in Chemical Engineering (2019) from the Massachusetts Institute of Technology. His research interests lie in the theory and simulation of nanomaterials, including their synthesis and applications for clean energy and water technologies. His group focuses on multi-scale modeling of electrochemical water splitting, catalytic carbon dioxide reduction, and membrane separations. He has served as a Guest Editor for ACS Engineering Au and the Journal of IISc. He is a Young Associate of the Indian National Academy of Engineering, an Associate of the Indian Academy of Sciences, and a recipient of the Amar-Dye Chem Award of the Indian Institute of Chemical Engineers.

IL-22: Computational Insights in CO₂ Capture and Conversion: An Industrial Perspective

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Abstract

Decarbonization of energy sector is one of the toughest challenges due to the large scale and complex nature of the processes involved in the conversion of carbon based feedstock. Considering the stringent policies for low carbon chemicals, its very critical for the energy industries to reduce the CO₂ footprint in their processes.¹ To tackle this, one needs to adapt novel materials that will efficiently capture CO₂ and convert that to useful chemicals. Several studies have been dedicated for designing new materials for CO₂ capture and conversions.² In recent years, computational methods in conjunction with machine learning algorithms have accelerated the design of novel materials for carbon capture and conversions.

In this presentation, I will provide the background on different industrial processes where CO₂ is captured and converted into sustainable chemicals and fuels. I will discuss the computational results on molecular mechanisms involved in the CO₂ capture on oxides and molecules and electrocatalytic conversion to CO.^{3,4} We have developed Deep Molecular Dynamics based potential to study deactivation of the supported Cu catalyst used for CO₂ conversion.⁵ Furthermore, I will conclude on the challenges and opportunities for technology development to achieve carbon net zero emissions.

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Dr. Sharan Shetty is a specialist in heterogeneous catalysis with expertise in Fischer-Tropsch synthesis, ammonia synthesis via the Haber-Bosch process, and the three-way catalytic (TWC) converter. His work primarily focuses on understanding molecular steps in key industrial processes through computational chemistry. He investigates CO activation, hydrogenation, and C-C coupling reactions on Ru and Co surfaces and nanoparticles, alongside the formation of ammonia on Ru surfaces and the NO reduction process in TWC. Additionally, his research explores the formation of C1 and C2 oxygenates on Rh clusters and methane decomposition on Ru surfaces, as well as reactions in zeolites like the Baeyer-Villiger oxidation in BEA-zeolite. Dr. Shetty is currently based at Shell Technology Centre in Bangalore, India.

IL-23: Role of Sorption-Enhanced Reactions in a Circular Carbon Industry

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Abstract

Sorption-enhanced reactions involving CO₂, which shift equilibrium favorably by in situ separation of a reaction product, enable CO₂ capture and utilization. They will significantly contribute to a circular carbon industry. In sorption-enhanced reaction processes, the removal of one of the products by in situ adsorption improves the conversion per pass of an equilibrium-limited reaction. Sorption enhancement improves product selectivity, catalyst stability and energy efficiency and reduces separation effort downstream of the reactor. This work focuses on the sorption-enhanced capture of CO₂ (reforming and chemical looping), sorption-enhanced conversion of concentrated CO₂ (sorption-enhanced methanation and sorption-enhanced reverse water-gas shift) and integrated capture and conversion of CO₂ over integrated catalyst-sorbent particles. These are promising options to revalue CO₂. The idea of sorption-enhanced reactions was applied in CO₂ capture and conversion to promote energy transition. Key challenges in sorbent regeneration, chemical stability and adsorption equilibrium require much research effort. This work will fast-track India's Panchamrita strategy (CoP26 policy) for net zero emissions by 2070 and advance the energy transition to a low carbon economy.

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Professor Prakash Vaidya is Rashtriya Chemicals and Fertilizers Chair in the Chemical Engineering Department at the Institute of Chemical Technology in Mumbai. He is an expert in catalysis, separations, and reaction engineering. He works in energy transition, especially promotion of carbon footprint reduction in the energy systems during the transition, e.g., by carbon dioxide capture and its chemical recycling, and improved production of hydrogen and biofuels. So far, he has authored 140 publications and 4 patents, and successfully guided 35 PhDs and 65 MTech scholars. He has been a Humboldtian, Liverpool University's India Fellow and Fellow of the Indian Chemical Society and Maharashtra Academy of Sciences.

IL-24: Multifunctional 2D Material-Based Sensors and Energy Harvesting Systems

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Abstract

Over 15 years after the first report of 2D material, Graphene and 2D material remain an active field of research considering their large surface area, excellent electrical and thermal conductivity, and abundance of catalytic sites in the field of electronic, photonic, sensing and energy harvesting. Although the layered structures demonstrate many beneficial attributes in this field, doping, functionalization, and patterning of these materials further open up a large area of research for enhancing sensitivity and active sites. Despite their potential, the challenge lies in fully harnessing these properties to develop multifunctional devices that can address complex real-world problems. One such challenge is the growing demand for advanced sensors for healthcare and environmental monitoring as well as efficient energy conversion systems towards sustainable energy solutions. Our research has been centered on advancing the application of 2D materials and graphene-based systems, with a focus on creating integrated solutions for sensing, energy harvesting, and environmental monitoring. We explore how various stimuli influence their electrical properties, discovering that chemical vapor deposition-grown SnSe flakes exhibit negative photoconductivity. This phenomenon is attributed to the adsorption and desorption of water and oxygen molecules at the edge active sites of SnSe. By etching the flakes along their most active planes, further enhancing their photodetection capabilities (Figure 1a). Additionally, its sensitivity to humidity has been harnessed to create a highly responsive humidity sensor, which can be utilized for monitoring human respiration—an important application in medical diagnostics.¹ To further enhance the utility of these materials, we have functionalized them with specific dopants, enabling their application in energy harvesting. SnSe, after functionalization, is used as an electrocatalyst in electrochemical hydrogen generation, showing improved catalytic performance with an overpotential decrease by several hundred millivolts. Furthermore, an on-chip microcell configuration facilitates the study of light and electric field effects on the catalytic properties and identifying the active catalytic sites. Parallely, we developed self-powered ultrafast sensors using nitrogen-doped graphene anchored with cobalt nanoclusters (Co-N-Gr) which exhibits triboelectric nanogenerators (TENGs) not only provide exceptional sensitivity for detecting NO_x levels in human respiration but also offer the ability to differentiate respiratory conditions, such as acute exacerbations of chronic obstructive pulmonary disease (AECOPD) (Figure 1b).² This work laid the foundation for exploring the broader potential of Co-N-Gr towards energy harvesting. The hydrophilicity and enhanced charge transfer capabilities of the such doped carbonaceous system allowed us to achieve a significant increase in power generation by 108 times, particularly in environments with varying pH levels and the presence of acidic contaminants. This seamless transition from sensing to energy harvesting highlights the versatility of 2D materials as multifunctional materials capable of integrating environmental monitoring, healthcare with sustainable energy solutions.

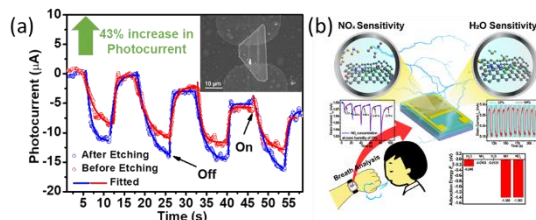


Figure 1. (a) SnSe flakes show increased photocurrent after being etched along the most active plane directions; (b) Co-N-Gr template being used for detecting NO_x levels and human respiration monitoring

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Prof. Kaushik Ghosh research interests are within the domain of developing advanced nanomaterials and nanocatalysis for Green hydrogen production typically in uninterrupted manner. His group is working on metal chalcogenides, phosphides & oxides on highly porous carbon matrix or impregnated inside the carbon shielded environment for harvesting solar energy followed by store it inside the energy storage device and finally transform it into the chemical form of renewable energy towards green fuel production. His group is also focused on industrial waste management for water purification as well as utilize this water and direct sea water for H₂ production via cost effective manner. He has developed 2D materials based sensor for health care monitoring as well as control its catalytic properties where he is trying to develop research on fundamental science drive towards innovation in applied technological perspective. He has achieved few awards including international researcher award 2024 from Meijo University Nagoya Japan.

IL-25: Hydrogen Production from Formic Acid Decomposition Over Supported Pd Alloy Catalysts: Role of Oxygen in Aqueous Phase Reactions

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Abstract

Formic acid (FA) is a potential liquid hydrogen (H_2) carrier due to renewable sourcing, low toxicity, and high H_2 density.¹ Supported Pd-Ag alloy nanoparticles are more reactive and selective than metals such as Pd, Au, and Ag for H_2 production from FA dehydrogenation.² However, the mechanism of aqueous FA reaction over Pd under aerobic conditions is still debated.³ Our study explains how Ag alloying of Pd and the crucial interfacial sites affects the selective production of H_2 from FA with rates, selectivities, and apparent energy barrier measurements without promoters in the liquid phase on different PdAg alloy catalysts supported on CeO_2 , TiO_2 , and Al_2O_3 . The catalysts were tested in a sealed round bottom flask with aqueous FA, and gases were quantified with a gas chromatograph. 0.5 PdAg- CeO_2 (atomic ratio of Pd and Ag is 0.5) catalysts provide higher H_2 selectivity and TOF when compared to Pd- CeO_2 . Ag alloying induces electronic changes in Pd due to the charge transfer from Pd to Ag, increasing the apparent activation barrier over 0.5 PdAg- CeO_2 than Pd- CeO_2 . The surface coverage of oxygen on Pd does not affect the H_2 production but rather the CO_2 production. The surface oxygen on Pd selectively oxidizes the CO formed from the FA reaction, thereby improving the catalyst stability. Similar-sized PdAg nanoparticles on CeO_2 and TiO_2 provide comparable rates of H_2 production from FA reaction despite the identity of the support due to negligible differences in the PZC of the supports. These mechanistic insights into FA reaction over supported PdAg nanoparticles will aid in rational catalyst design for selective H_2 production.

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Prof. Abinaya Sampath got her B.Tech (Hons.) in Chemical Engineering at IIT Madras in 2016. She obtained her Ph.D. in Chemical Engineering from the University of Illinois at Urbana-Champaign in 2022. During her doctoral studies, she worked on using surface science studies in ultra-high vacuum and *in situ* Raman spectroscopy to understand selective bond activation over heterogeneous catalysts. Abinaya Sampath joined IIT Gandhinagar as an Assistant Professor in 2022, soon after her Ph.D., and is working on using *in situ* and *operando* techniques to study the oxidation of bio-derived molecules for hydrogen production.

IL-26: Catalytic Nano-devices for Sustainable Chemical Synthesis

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Abstract

We design and synthesize multicomponent nano-architectures, translating to the unique optoelectronic and catalytic properties. These ‘nanodevices’ integrate active-sites with plasmonic/magnetic-antennae in a compartmentalized nanospace, with the objective to control molecular reactions’ selectivity, which otherwise are elusive with conventional thermal heating conditions. Remotely operating light and/or magnetic field as energy source, highly efficient and nano-localized interfacial energy-flow with distinct photocatalytic or charge-transfer pathways are possible individually, on proximal active-sites. Such catalyst designs endow independent control of reaction-steps and desired selectivity outcomes. With the potential to perform new-to-nature reactions, these catalysts as nanodevices, can be easily coupled with the living cells and microorganisms for sustainable biorthogonal and chemobiotic cascade catalysis.

We also develop ‘model-nanocatalysts’ consisting of tunable surface-microenvironments on well-defined metal atomic-arrangements, to address the challenge of studying and controlling random molecular adsorption/desorption behaviors. Ultrathin silica, polymer or covalent organic overlayers having molecular scale porosity and interlayer nanospaces in conjunction with the ligand-additives provide well-engineered ‘electronic’ and ‘geometric’ effects. Such complexity-by-design approach provides wealth of mechanistic information regarding to the presence of intermediates, coordination modes, and molecular orientations by employing in situ reaction monitoring techniques.

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Amit Kumar received his M.Sc. (Chemistry) degree from IIT Roorkee in 2004 and Ph.D. (Organic Synthesis) from IIT Kanpur in 2009, followed by post-doctoral research from City University of New York (USA) and Seoul National University (S. Korea). He is currently working as Research Professor in the Department of Chemistry POSTECH (S. Korea) and supervising PhD students and post-docs as associate group leader. His major research interest is to design and synthesize advanced functional nanostructures by focusing on new nanoscale solution-phase and solid-state materials chemistry and to apply them in different fields: stimuli-responsive (plasmonic/magnetic) catalytic nanoreactors, sustainable chemical synthesis, chemically-fueled nanomotors, photocatalysis and biorthogonal catalysis. His impactful research has been published in esteemed research journals like Nature Communications, Advanced Functional Materials, JACS, Angewandte Chemie, ACS Nano, Nano Letters etc.

IL-27: Enhancing The Performance of Rechargeable Flexible Batteries

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Abstract

The performance of a rechargeable metal air battery largely depends upon the performance of bi-functional oxygen electrode. The oxygen reduction reaction (ORR) during discharging and oxygen evolution reaction (OER) during charging play crucial role for the same. The major constraints that limit the performance of metal air batteries are the sluggish kinetics of oxygen evolution reaction (OER) and oxygen reduction reaction (ORR) where the issues of overpotential as well as stability at higher voltage are highly prevailing. In this work, the working mechanism of overall flexible and reversible-ZABs and the problems associated with cathode, anode, and electrolyte will be discussed. This talk will also be focused on discussing how different strategies like doping, hetero-junction formation, morphology control, oxygen vacancy creations etc could be adopted to improve the performances of these reactions.

Additionally, I will also address how we have utilized and explored layered oxide materials for fabricating bifunctional electrode material. The designed materials have also been explored for influence of photoactivity on energy storage ability. Four different strategies, 1) doping, 2) co-doping, 3) allomorphous synergism and 4) photoactivity will be explained for the performance enhancement for the same. The research work carried out in our group indeed confirms that all these strategies singularly or in combination are capable of enhancing the performance of energy storage devices.

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IL-28: On Assessing the Carbon Capture Performance of Graphynes with Swarm Intelligence

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Abstract

Tackling climate change is one of the greatest challenges of current times and therefore the development of efficient technologies to limit anthropogenic emissions is of utmost urgency.¹ Recent research towards this goal has alluded to the use of carbon-based solid sorbents for carbon capture. Graphynes (GYs), an interesting class of porous carbon membranes, have recently proven their potential as excellent membranes for gas adsorption and separation.²⁻⁴ Herein, we explored the CO₂ and N₂ adsorption characteristics and CO₂/N₂ selectivities of a class of GYs, namely γ -GY-1, γ -GY-2, and γ -GY-4. We investigated the putative global minimum geometries of adsorbed unary ($n=2-10$) and binary ($n:m$; $n, m \in [1,8]$) clusters of CO₂ and N₂ by employing a stochastic global optimization method called particle swarm optimization in conjunction with empirical intermolecular force field formulations.⁵⁻⁸ The intervening interactions are modeled using various pairwise potentials, including Lennard-Jones potential, improved Lennard-Jones potential, Buckingham potential, and Coulombic potential.⁹ The binding energies for both unary and binary clusters are the highest for adsorption on γ -GY-1, followed by γ -GY-2. The putative global minimum geometries suggested that N₂ molecules preferred binding over the pore centers while CO₂ molecules showed higher clustering propensity than any binding site preference. The predicted energetics suggested higher selectivity for CO₂ over N₂ for all the three γ -GYs.

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Dr. R. S. Swathi's research focuses on providing a fundamental understanding of various chemical systems and phenomena involving carbon-based and metal-based nanostructures using the methods of theoretical chemistry. Her group employs analytical and computational approaches for their research explorations on the utility of nanostructures for sensing, storage, separation, and spectroscopy applications. Swathi is a recipient of the Young Scientist Awards from Indian National Science Academy, National Academy of Sciences, Kerala State Council for Science, Technology and Environment, and Distinguished Lectureship Award from the Chemical Society of Japan. Swathi was also a young associate of the Indian Academy of Sciences, Bangalore. Swathi is a recipient of the A. V. Rama Rao Foundation Prize in Chemistry awarded by the JNCASR, Bangalore for the year 2020. She is currently an editor of the journal *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, published by Elsevier, and an associate editor of the journal *Bulletin of Materials Science*, published by the Indian Academy of Sciences, Bangalore. Additionally, Swathi serves on the editorial advisory board of *ACS Applied Optical Materials*.

IL-29: Catalytic Processes Using CO₂ for the Chemical Value Chain: Catalyst Formulation by Developing Structure-Activity Relationships

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Abstract

There is ample scope of catalytic process innovation for chemical, petrochemical and refinery industries by utilizing CO₂. The challenge lies on effective catalyst design followed by overall process development. Essentially, chemical conversion of CO₂ into useful products is important to minimize climate change effects and among the notable reactions which demand effective catalyst design are, (i) CO₂ reforming of Methane (DRM), (ii) Methanation of CO₂ (Sabatier Reaction), and (iii) Oxidative dehydrogenation of propane (ODHP-CO₂). In this talk, using catalytic reaction engineering principles we have formulated transition Non-noble metal based alloy catalysts for DRM and Methanation reactions.

Bimetallic Ni-Co alloy catalyst exhibits better activity than Ni, Ni-Fe and Ni-Cu alloy catalysts.^{1,2} To understand the intrinsic kinetics, we performed DFT calculations and established descriptors for activity and stability^{3,4} Addition of Boron to Ni-Co alloy further improves catalyst stability by competing with carbon on the surface sites of Ni-Co alloy catalyst.⁵ Interestingly, oxygen vacancy formation energy correlates with oxygen storage capacity for Ceria based DRM catalysts.⁶ On the contrary, Ni-Fe alloy catalyst outperformed other Ni-based catalysts and showed interesting alloy properties as obtained from DFT study.⁷ This catalyst can compete with Noble metals (Rh, Ru) as there exists a volcano relationship between dissociative CO₂ adsorption energy and TOF_{CO₂}.⁸ Very recently Cr-based mixed metal oxides are exhibiting interesting catalytic activity than Cr alone for propane dehydrogenation. We are extensively carrying out experiments to check what catalytic effects it can offer to ODHP-CO₂, a very promising reaction of recent times.

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Prof. Koustuv Ray research interests primarily include gas phase catalysis for alkane and CO₂ activation and transformation into value-added chemicals and fuels. The work of his group focuses on developing structure-property and structure-activity relationships, deriving intrinsic kinetics for catalyst screening and revealing key mechanistic insights by combining the knowledge of steady state kinetics, *in-situ* FTIR spectroscopy (DRIFTS) and First-principle based DFT calculations. His other research interests are Photocatalysis, Biohydrogen production and combining DFT with Machine Learning for catalyst prediction. His passion includes playing football, watching football matches, and photography.

IL-30: AI-Driven Discovery of Asymmetric Pauson-Khand Reactions: A New Toolbox in a Synthetic Chemist's Treasure

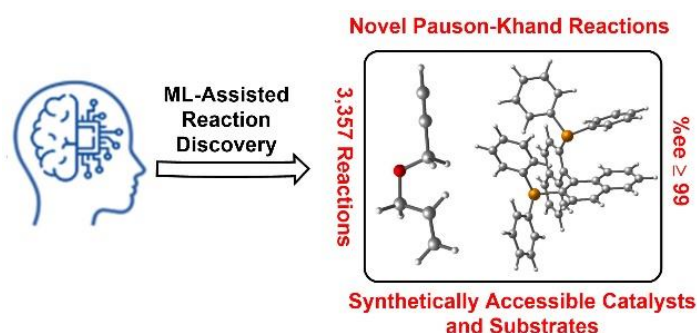
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Abstract

Asymmetric Pauson-Khand reaction is widely used for synthesis of enantiopure five-membered cyclopentenone which is an essential building block for construction of complex molecular architectures with high stereochemical precision.¹ However, the enantiomeric excess (%ee) obtained in this reaction is significantly impacted by both the structural complexity of substrates and catalysts and the reaction conditions like temperature, solvent polarity, and CO gas pressure.^{2,3} A direct correlation between the reaction output (%ee) and the molecular/non-molecular descriptors is still unknown even in today's date which is a significant challenge for judicious reaction design. In the present study, we have used a robust machine learning model and discovered a library of 3,357 new Pauson-Khand reactions by engaging experimentally unknown combinations of the catalysts, substrates, and reaction conditions. These new reactions have been predicted to have %ee ≥ 99 . Four different machine learning algorithms have been used: extreme gradient boosting, random forest, light gradient boosting machine, and neural network. The axially chiral biaryl catalysts and 1,6-enyne substrates, present in our library, is synthetically accessible. Our machine learning model with high throughput %ee prediction can be of great help in designing reactions from scratch without extensive experimentation, thus saving manpower, energy, money, and generation of chemical waste.



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Dr. Shivnath Mazumder is an Assistant Professor at the Indian Institute of Technology (IIT) Jammu, specializing in computational molecular modeling and catalysis. His research interests include bio-inspired multi-electron catalysis, artificial photosynthesis, molecular electronics, and metal-catalyzed coupling reactions for drug discovery. Dr. Mazumder's work focuses on designing sustainable catalysts for critical chemical transformations, such as C-H activation and water splitting, leveraging computational and theoretical approaches to drive innovation in green chemistry. Dr. Mazumder has received prestigious grants, including one from the Royal Society of Chemistry for automated discovery of sustainable C-H activation catalysts, and has published extensively in high-impact journals like *Angewandte Chemie International Edition* and the *Journal of Physical Chemistry C*. His research group's achievements include novel insights into reaction mechanisms and catalyst design, recognized through awards and cover articles in reputed journals.

IL-31: Toward a Carbon-Neutral Energy Economy via Recycling CO₂

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Abstract

In the context of rising CO₂ concentration in the atmosphere and the detrimental effects it is having on the biosphere, use of alternative fuels which can offer a low-carbon or carbon-neutral pathway for storage and utilization of low-carbon energy by maintaining the net atmospheric CO₂ concentration might be a prospective solution. Among the wide variety of CO₂-reduced products, formic acid (HCO₂H), formate salts (HCO₂M; M = Na, K), and methanol (CH₃OH) are particularly important due to their ability to be used as alternative fuels or a reversible H₂-storage and H₂-carrier material. For the past one decade, our group has been actively engaged in developing molecular homogeneous as well as single-site heterogenized catalysts for thermochemical and electro/photochemical CO₂ reduction to the above value-added products, coupled with integrated CO₂ capture processes.¹⁻⁷ Our focus is mainly concentrated on “hydride-transfer”-based mechanistic pathway for driving the catalytic “CO₂-to-fuel” processes. This talk will illustrate the above chemistry in detail, and will emphasize our research in this important field.

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Joyanta Choudhury obtained Ph.D. in 2006 from IIT Kharagpur, India working under Professor Sujit Roy on the development of Ir-Sn heterobimetallic complexes for aromatic C–H functionalization. He then moved to The Scripps Research Institute, Florida, USA for postdoctoral work with Professor Roy A. Periana in the field of CH₄-to-CH₃OH (MTM) conversion chemistry. In 2008, he received Marie Curie International Incoming Fellowship from the European Union and went to the Weizmann Institute of Science, Israel to work with Professor Milko E. van der Boom on redox-active molecular assemblies on solid surfaces. He joined the Department of Chemistry, IISER Bhopal, India in 2011.

His research group at IISER Bhopal works primarily on (a) developing new reactions involving “metal-NHC” intermediates for the creation of task-specific functional molecules, (b) circular catalysis with CO₂, H₂ and biomass-derived energy carriers toward alternative fuels, and (c) reversible energy storage and delivery. Some of the research findings on CO₂ conversion from his laboratory have been critically acclaimed through several commentaries, essays, previews etc. in leading popular science magazines and journals such as *ChemistryWorld* ((a) [Helicenes are the ‘first true organic electrocatalyst’ for carbon dioxide reduction | Research | Chemistry World](#); (b) [Taking the pressure off catalytic carbon dioxide conversion | Research | Chemistry World](#); (c) [Ruthenium complex catalyses complimentary reactions | Research | Chemistry World](#)), *Joule* ([Metal-free molecular catalysts for electrochemical CO2 reduction - ScienceDirect](#)) etc.

Award: Chemical Research Society of India, Bronze Medal (2019)

IL-32: Valorization of CO₂

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Abstract

The evanescent nature of existing carbon-based fossil fuels, paired with excessive anthropogenic release of CO₂ have spurred research efforts towards not only on carbon capture, but also on reduction of CO₂ to obtain clean fuel.¹ A significant research effort is underway across the globe to reduce CO₂ to valuable products as a road map of Net Zero emission. Thermocatalytic transformations of CO₂ predominately involve Dry Reforming of Methane (DRM). The electrocatalytic reduction of CO₂ (CO₂RR) with renewable energy is advantageous as the process uses water as the hydrogen source instead of molecular H₂. The photocatalytic reduction of CO₂ (PCR) on other hand is also a potential sustainable technique to produce value-added chemicals and green fuel feedstocks. This presentation will narrate our effort towards exploring the CO₂ - valorization techniques. Our studies on DRM over defect fluorite La_{2-x}Sr_xCe_{2-y}Ni_yO_{7-δ} sheds light on the importance of designing efficient DRM catalysts to optimize syngas production and prevent carbon fouling. A series of MOF derived nano-alloys synthesized in our laboratory, such as Pt_xZn/C, Cu_{1-x}Ni_x/C and Cu_{1-x}Zn_x/C demonstrated high structure dependency as well as unique electronic properties towards the CO₂RR to value added products.²⁻⁴ Also, the photocatalytic reduction of CO₂ over Ce-based semiconducting MOFs exhibited the significance of the band energetics of the materials and the relative position of the reduction potentials.

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Sounak Roy is professor at BITS Pilani, Hyderabad Campus. After completing his doctoral programme at IISc Bangalore, he pursued postdoctoral research at ETH Zurich and the University of Pennsylvania before starting his independent career at BITS Pilani, Hyderabad Campus. His research focuses on heterogeneous catalysis for sustainable energy and environmental solutions, as well as solid-state chemistry. He is particularly interested in exploring the structure and surface properties of solid materials for catalytic applications.

He is an elected Fellow of Telangana Academy of Sciences (2021) and Royal Society of Chemistry (2023). He is a recipient of Society for Materials Chemistry (SMC) Bronze Medal (2024) and also a visiting international Professor of Ruhr-Universität Bochum (RUB), Germany (2024 - 2025).

IL-33: CO₂ to Value-Added Polycarbonate Diol

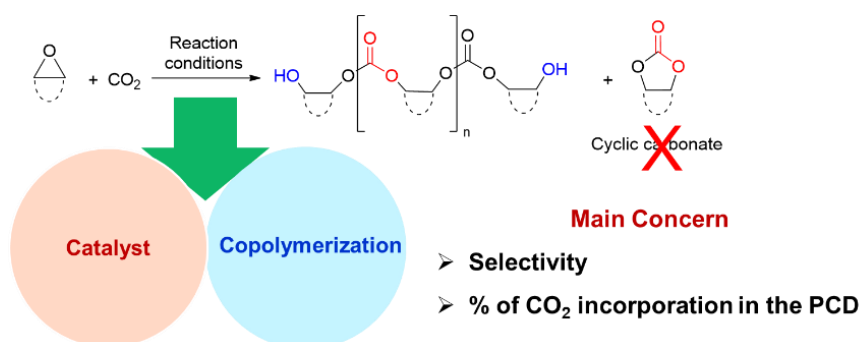
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Abstract

Carbon dioxide (CO₂) as an abundant, non-flammable, economical, and renewable C1 feedstock is of strategic importance for our dependence on depleting non-renewable fossil derivatives. One of the most attractive areas of CO₂ utilization is its direct application as a renewable raw material for polymer synthesis, as large amounts of CO₂ can be utilized to make value-added polymeric products.¹ Polycarbonate has a terminal hydroxyl group (polycarbonate diol; PCD) plays a role in its excellent adhesive properties. The primary application of low-molecular-weight polycarbonate diol is widely used as an intermediate in the production of polyurethane (PU) foams. PCD-derived polyurethane has both financial and environmental benefits. The present work mainly involves the development of efficient, scalable catalysts for the production of PCD with excellent selectivity as well as tunable molecular weights and enhanced CO₂ incorporation.² The production of polycarbonate diol will be achieved at ambient temperature and low pressure of CO₂. This process may open varied opportunities and emerge as a game-changer technology for engineering polyurethane foams.



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Dr. Ekambaram Balaraman's research primarily focuses on generating resources for green energy and recycling atmospheric waste. Specifically, he works on the design and development of catalytic materials for hydrogen generation from feedstocks, sustainable chemical synthesis, and conversion of CO₂ to value-added products. He is also interested in the development of electron donors for heterogeneous Ziegler catalysts used in the manufacture of isotactic polypropylene. Dr. E. Balaraman received his M.Sc in Chemistry from R.K.M. Vivekananda College, Chennai (2002), and Ph.D from the Central University of Hyderabad (2008). Subsequently, he has been an FGS-Post Doctoral Fellow at the Weizmann Institute of Science (2008-2012). In July 2013, he started his independent career as a senior scientist at the CSIR-National Chemical Laboratory. In Dec'2018, he moved to the IISER-Tirupati as a faculty in chemistry. He is the recipient of the MRSI Medal (2021), SwarnaJayanti Fellowship (2020), CRSI-Bronze Medal (2020), The Asian and Oceanian Photochemistry Association (APA) for Young Scientist (2019), Fellow of the Royal Society of Chemistry (2019), AV Rama Rao (AVRA) Young Scientist Award (2018). He is a member of the Indian National Young Academy of Science (INAYAS), INSA (2018).

IL-34: Chemistry and Materials from India's past: Illustrations and Contemporary Challenges

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Abstract

Materials, chemistry and metallurgical processes were no alien subjects to ancient humans across the globe with India being no exception. Given the uniqueness of India's geography, predisposed with the gift of a tropical climate and diversity of minerals ancient Indians left no stone unturned when it came to putting materials to their best use yet not at the cost of the environment. From artefacts of day-to-day use to medical formulations to manage/cure diseases chemistry flourished in a very pragmatic manner. Notwithstanding their contribution to our scientific heritage, they are relevant in contemporary times as a few of them defy our current understanding of materials using the modern chemical principles. Solubility being one such fundamental property which gets defied by an iron based traditional formulation. In this talk I will give an overview of such materials, talk about their conventional uses and discuss the contemporary challenges that such materials from our past pose to the modern understandings. Synthetic food colorants like Rhodamin 6G, Allura red, Amaranth, Tartrazine, and Sunset yellow although banned by several governments continues to be used in food products. A method for detection in a non-invasive label free manner is reported in two parts. Herein, a novel CTAB assisted-BiOBr (BOB), Ag 0.09 BOB and Ag 0.15 BOB (CTAB-AgBr-Bi₃O₄ Br/BiOBr) substrate was prepared by chemical precipitation method and their SERS (surface enhanced Raman spectroscopy) activity was assessed by detecting the aforementioned synthetic food colorants in a non-invasive label free manner. Excellent SERS activity was observed for all these dyes. Ag 0.15 BOB substrate showed higher SERS activity than others. The lowest detection limit was determined to be 10 μ M for Rhodamin 6G, 50 μ M for Allura red, Amaranth and 40 μ M for Tartrazine and Sunset yellow. Binary mixture analysis was also performed to analyse the closely related food colorants paving way for their quantitative detection in real food products.

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Dr. V. Ramanathan is a physical chemist working in the Department of Chemistry at IIT(BHU) Varanasi. He carried out his post-doctoral research works in University of Stuttgart in Germany, University of Basel in Switzerland and Seoul National University in South Korea. He obtained his PhD in physical chemistry from IIT Kanpur, India. His areas of academic research are Raman imaging and spectroscopy, Laser spectroscopy and computational chemistry. His other research interest lies in studying the scientific heritage of India, Indian traditional medicine, classical music and languages of India (comfortable in 7 Indian languages). He is a Fulbright scholar and a former core committee member of Indian National Young Academy of Science (a body of Indian National Science Academy (INSA)). His other professional engagements are:

- ☐ Chairman, Position Paper on Knowledge of India (NEP 2020), DSERT Govt. of Karnataka
- ☐ Member, National CAG for Science and IKS (NEP 2020)
- ☐ Member, Research Council for History of Science Indian National Science Academy
- ☐ Member, Curriculum development and NET exam syllabus committee of UGC in IKS
- ☐ Chairman, UGC-NET paper on IKS
- ☐ Science Textbook Writing Team Leader, SAMVIT Bengaluru (NGO specialized in school textbook writing)
- ☐ Member, Advisory Council and Board of Studies, Mahayogi Gorakhnath University, Gorakhpur, U.P.

IL-35: Computational Advancement towards Efficient Catalytic Materials: Connecting a Few Dots

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Abstract:

In this talk, I would like to present a **two-fold** research activity interconnected with a common string “**Catalysis**”. I will start with the brief introduction of electronic structure calculations based on density functional theory (DFT) formalism, and how it could be connected to the computational screening for achieving highly efficient energy materials. The first part would be dedicated to the fundamental mechanism for the solar irradiated water splitting in *photocatalytic materials* with the future prospect of Non-linear Poisson Boltzmann Solver development for the heterogenous catalytic mechanism. The relevant exploration of novel 2D materials and their applications in such catalytic mechanism would be elaborated subsequently. The mechanism corresponding to Hydrogen Evolution Reaction (HER) and Oxygen Evolution Reaction (OER) under the influence of doping and vacancy defect from DFT based theoretical perspective would be discussed along with our recent high throughput computational investigation of finding efficient HER catalytic materials based on transition metal tri-chalcogenides. The next part of the talk would be devoted to the fundamentals and possible implications of Rashba phenomena in non-centrosymmetric structural materials and how it could govern the enhancement of catalytic efficiency, with an example case-study of BiClS janus monolayer for Hydrogen Evolution Reaction (HER) activity. We have recently successfully demonstrated the effect of strain on the overpotential of the novel catalytic materials through the tuning of Rashba splitting under the influence of external strain.

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Dr. Sudip Chakraborty is leading Materials Theory for Energy Scavenging (MATES Lab) group in India's premier theoretical research Institute Harish-Chandra Research Institute (HRI) Allahabad (Prayagraj), Department of Atomic Energy, Govt. of India. After completing his Ph.D. in collaboration between Bhabha Atomic Research Centre (BARC) and University of Pune, India, he moved to Max Planck Institute, Düsseldorf, Germany in March, 2011 as a Max Planck Postdoctoral Fellow. In February, 2013, he joined Materials Theory Division, Uppsala University, Sweden as a Förskares (Senior Researcher). Since March, 2019, he started leading his group firstly in Department of Physics of IIT Indore and later on in HRI from May, 2021 onwards. He has been awarded the Rising Stars by ACS Materials Au 2021, among 300+ nominations worldwide, while he is the sole recipient from India. He is in the Editorial Board of Journal of Physical Chemistry A/B/C (ACS), Energy Advances (RSC), Electronic Structure (IOP), Chemistry of Inorganic Materials (Elsevier) and Graphene & 2D Materials (Springer). His works are appeared in Nature Materials, PNAS, Materials Today, ACS Energy Letters, JACS, ACS Nano, ACS Catalysis, AngewChemie, Advanced Materials, Advanced Functional Materials, Chem.Mat. etc. He has 174 International publications with total 6500 citations and 45 h-index.

(https://scholar.google.com/citations?hl=en&user=ybAcs3kAAAAJ&view_op=list_works&sortby=pubdate)

IL-36: Role of Radical and Organometallic Pathways in Pincer-Metal Catalysis for Generation of Hydrogen, Fuel & Specialty Chemicals

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Abstract

Current global research is greatly focused on the development of greener, sustainable and atom-economical methods for the formation of C-C bonds leading to versatile fuels and value-added chemicals.¹ This greatly negates the typical disadvantages of classical coupling of alkyl halides that generally are accompanied by the formation of hazardous waste. Well explored approaches towards greener and sustainable C-C bond forming reactions involve catalytic C-X (X = H, Cl, Br, I) activation and subsequent cross coupling either involving radical mechanisms² or purely organometallic mechanisms.³ Transition metal catalyzed coupling of alcohols is a promising route to new C-C bonds as they are greener and atom-economical with water as the sole by-product.

For efficient catalysis, it would be desirable to have a subtle balance between catalyst stability and reactivity.⁴ For nearly five decades now, it has been more often found, that pincer-metal complexes perform exceedingly well in striking this balance.⁵ With a particular emphasis on base metals, the current talk would provide a glimpse on the pincer chemistry that is being investigated in our lab, while shedding light on their role in catalyzing C-H activation/functionalization mediated C-C bond formation of alcohols via radical/organometallic pathways that ultimately lead to synthesis of hydrogen, high value fuels and specialty chemicals starting from waste.⁶

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Dr. Akshai Kumar has about 20 years of experience in the area of organometallic chemistry, homogeneous catalysis and heterogenization of molecular catalysts. He has 60 research articles in peer-reviewed journals, including one in Chemical Reviews (Impact Factor = 54. 301) apart from 6 book chapters and 4 US patents (granted), 1 INDIAN patent (granted), 6 International patents (filed) and 6 INDIAN patents (filed). Career highlights include the development of efficient catalyst for transformation of waste to fuel and value-added chemicals. This includes conversion of unproductive hydrocarbons to fuel-grade chemicals, upgrading low-energy density ethanol to high-energy density fuels and generation of green hydrogen via transformation of inexpensive glycerol, ethanol and methanol to high value lactic acid, acetic acid and formic acid respectively. He is a member of Indian Young Academy of Science, Member of Bureau of Indian Standards, and fellow of the Indian Chemical Society. In addition to Associate Professor at the Department of Chemistry, currently, he is the Head, Centre for Nanotechnology at IIT Guwahati.

IL-37: Designing Catalysts and Reactors for Enhancing Scalability

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Abstract

Heterogeneous catalysis forms the backbone of chemical industry, from early days when Ni was used in edible oil industry, later being prevalent in petroleum industry. Focus of chemical industry last century may have been productivity, but current challenges of pollution and consequent effects have shifted the focus to include product selectivity and sustainability. Even though multitude of novel materials are reported for various transformations, scaling up is still challenging, delaying deployment of new technologies. Simple approaches can be taken to ensure scalability of catalytic processes.

I will present few examples whereby multiprong approaches have contributed in increasing selectivity and scalability in commercially interesting chemical processes. Novel reactor design has helped us in improving selectivity in CO₂ conversion processes. Integrating separation into some of the catalytic processes also enhance selectivity to desired products. Similarly, incorporation of optical fibers for photocatalysis enhances the scalability compared to traditional modes.

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Dr. R. Nandini Devi is a distinguished researcher specializing in the synthesis of noble metal clusters, nanoparticles, and structured oxides with applications in bioimaging, catalysis, and energy. Their work focuses on developing sinter-resistant catalysts for the Water Gas Shift Reaction in hydrogen generation, disordered oxides for gas separation, and innovative materials for solar energy harvesting. Dr. R. Nandini Devi earned their PhD (2000) and MSc (1994) in Chemistry from the Indian Institute of Technology Madras, Chennai. They have held prestigious postdoctoral positions at Syracuse University, USA, the University of St. Andrews, UK, and Queen's University Belfast, UK, collaborating with eminent researchers like Prof. J. A. Zubieta, Dr. P. A. Wright, and Prof. R. Burch.

IL-38: Towards Rational Design of Transition Metal Catalysts for the Upgradation of Biorenewables

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Abstract

Biomass is a renewable and sustainable source of carbon and is a promising alternative to produce fuels and chemicals. Efficient catalytic system is crucial for enhancing the utility of biomass derived platform compounds. Our research is based on the utilization of density functional theory (DFT) simulations to design transition metal-based catalysts for different reactions such as hydrogenation, ring-opening, hydrodeoxygenation, etc. involved in the upgradation of biomass derived platform molecules to value added fuels and chemicals¹⁻³. Further metal/solvent interface plays a key role in the catalytic upgradation of biomass derived platform molecules. The type of solvent used affects the kinetics and thermodynamics of the reaction, thereby altering the conversion and selectivity. By combining ab-initio Molecular Dynamics (AIMD) with DFT simulations a fundamental understanding on the solvent effect in hydrogenation reactions involved in biomass conversion is being developed.

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Dr. Shelaka Gupta research interests are focused on both experimental and theoretical heterogeneous catalysis for sustainable production of fuels and chemicals. Her research group uses quantum mechanical ab initio density functional theory (DFT) simulations for the rational design of heterogeneous catalysts used for the sustainable production of fuels, materials and chemicals. The ab initio calculations provide a mechanistic insight of the reaction which helps in engineering the catalyst. She has been recognized as India's 75 women in STEAM by the Office of Principle Scientific Adviser to the Government of India in the year 2022. She is also a recipient of Sumant Sinha Sustainability Leadership Award (2019) and Gandhian Young Technological Innovation (GYTI) Award (2018). She is a co-founder of WowChemE Pvt Ltd. at IIT Delhi, which is focused on commercializing biorenewable products.

IL-39: Green Hydrogen Generation: A Step Towards Net Zero Emissions

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Abstract

For curbing the carbon emissions in environment, employment of non-carbonaceous fuel to fulfil our energy demands is one of the potential alternatives towards clean energy. Hydrogen generation from water splitting using renewables is one of the most sought-after option [1-4]. For clean and green hydrogen production via water splitting, the electrolyzers are in fore front and are leading the green hydrogen campaign. Water electrolysis via alkaline or PEM based electrolysis although demonstrated to have potential for large scale hydrogen production, but suffers from corrosive environment, high cost of noble metal based electrocatalysts and imported membranes are deployed in membrane electrode assemblies. Alternative methods are thermochemical hydrogen production, photocatalytic or photobiological processes. Thermochemical hydrogen production using iodine-sulfur and copper-chlorine thermochemical processes have potential for large scale hydrogen production using nuclear source of energy. Processes such as photocatalytic and photoelectrochemical are at R&D stage and are in search of visible light active, robust and sustainable photocatalysts with at least 10% solar to thermal efficiency. Present talk will deliberate about merits and demerits of different hydrogen production processes with respect to process efficiency, materials, economic viability, proof of concept and the scale of operation. R&D on catalytic materials, reaction kinetics and mechanism of various steps for iodine-sulphur and copper-chlorine thermochemical water splitting processes will be discussed. A few studies on next generation conjugated photocatalytic materials (carbon nitride, MOF, COF-based photocatalysts) will also be discussed with emphasis on light harvesting properties, interfacial charge transfer kinetics, band alignment and photocatalytic hydrogen yield.

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IL-40: Computational Catalysis for Sustainability: Fuels from CO₂ and Methane

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Abstract

Advanced computational modeling techniques, such as Density Functional Theory (DFT), provide a powerful approach for studying chemical and physical interactions at the molecular level and enable the design of novel materials that can meet future energy demands sustainably. In this talk, I will discuss two key areas: methane pyrolysis in molten media and the catalytic conversion of CO₂ into value-added chemicals. Methane pyrolysis in molten media is an emerging technology for producing CO₂-free hydrogen and solid carbon. However, molten salts generally exhibit weak catalytic activity. This study explores catalytically active molten media by dispersing solid metal in molten salt for methane pyrolysis, yielding hydrogen and valuable C₂ products. Additionally, with the growing concerns over CO₂ emissions and their environmental impact, converting CO₂ into fuels and value-added products is becoming increasingly important. However, designing efficient catalysts remains a challenge. We address this challenge using DFT-based simulations, although they are computationally expensive. To mitigate this, we demonstrate the integration of Machine Learning with DFT to predict activation barriers for CO₂ conversion reactions efficiently.

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IL-41: Perturbing a Chemical Equilibrium through Vibrational Strong Coupling

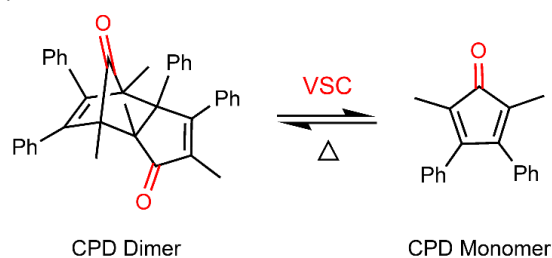
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Abstract

Light-matter strong coupling, in general, and vibrational strong coupling (VSC), in particular, offer an exciting and innovative approach to controlling molecules' chemical reactivity.¹ In the strong coupling regime, molecular vibrations are resonantly coupled with the confined electromagnetic field, generating hybrid vibro-polaritonic states through coherent energy exchange. The presence of such light-matter hybrid states in the molecule has proven to modify various physicochemical properties of the materials. A handful of chemical reactions have been reported under VSC conditions to modify the reaction rate, chemical equilibria, chemo-selectivity, and stereo-selectivity.²



Here, we attempt to understand the impact of VSC on the chemical reactivity of a cyclopentadienone (CPD) derivative. CPD derivatives form dimers at room temperature and dissociate into their monomers at elevated temperatures.³ It is well known that the carbonyl group and other substituents in the CPD derivatives can manipulate their chemical reactivity.³ In this work, we strongly couple their carbonyl stretching to the Fabry-Perot cavity modes to study the impact of VSC on the monomer-to-dimer equilibrium of the given CPD. The results indicate that the VSC can alter the CPD derivative's chemical reactivity and perturb the abovementioned equilibrium.⁴

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Dr. Kalaivanan Nagarajan's research interests include understanding the physics and chemistry of materials under light-matter strong coupling conditions. His research group explores the possibility of using vibrational strong coupling (VSC), where molecular vibrations are strongly coupled with the confined electromagnetic modes, to tune the chemical reactivity of the coupled molecules. Since 2022, he has been a Reader in the Department of Chemical Sciences, Tata Institute of Fundamental Research Mumbai, leading the Light-Matter Hybrid Chemistry Lab (LMHCL).

IL-42: Development of Efficient Heterogeneous Catalysts for Sustainable Plastic Upcycling, Biomass Valorization, CO₂ Conversion and Transfer Hydrogenation Reactions

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Abstract

Energy crisis and environmental deterioration has emerged as major problems around the world in recent times, mainly due to combustion of fossil fuels and their depletion. The utilization of light and thermal energy to produce chemical fuels is an attractive and major strategy to address the global energy crisis and other environmental issues. Our research group has recently developed several two-dimensional materials supported nanostructured photocatalysts based on semiconductors, plasmonic materials, perovskite structures and upconversion nanoparticles for energy generation and environmental remediation applications. In addition to photocatalytic hydrogen generation, nitrogen fixation and pollutants degradation, our group has also utilized these materials for plastics upcycling biomass valorization, carbon dioxide conversion and Green organic transformations, either by functionalization or doping with a heteroatom. The highlights of the ongoing research work of our group will be presented.

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Prof. Venkata Krishnan completed his Ph.D. in Chemistry in 2006 from University of Stuttgart, Germany after completing his B.Sc. and M.Sc. degrees from PSG College of Technology, Coimbatore, Tamil Nadu, India. Subsequently, he worked as a postdoctoral researcher at University of Pennsylvania, U.S.A. from 2006 to 2010 and then as a research associate at National Institute for Materials Science (NIMS), Tsukuba, Japan from 2010 to 2012. He joined as a faculty at the Indian Institute of Technology (IIT) Mandi in April 2012 and is currently a full professor. His research group is mainly working in the field of Green Chemistry and Heterogeneous Catalysis for Energy and Environment Applications. He has successfully guided 12 Ph.D. and 26 M.Sc. students and is currently guiding 8 Ph.D. and 7 M.Sc. students, in addition to several short-term research interns. He has published more than 180 articles in well reputed international journals and is also a reviewer for several scientific journals. He has been bestowed with several awards, including DST INSPIRE faculty award, IIT Mandi foundation day award for excellence in teaching, MANA research fellowship, DoE postdoctoral fellowship, DFG doctoral fellowship, DAAD visiting scholar fellowship, etc. In addition to teaching and research, he has also served IIT Mandi in various administrative positions, such as first warden of the main hostel in permanent campus, founding coordinator of Advanced Materials Research Center (AMRC), Associate Dean Research and most recently as Dean of Sponsored Research, Industrial Consultancy, and International Relations (SRIC & IR), Director of IIT Mandi iHub and HCi foundation (a technology innovation hub) and Director of IIT Mandi Catalyst (a technology business incubator), besides being on several scientific and administrative committees at institute, national and international levels. Apart from academics, he likes reading books and is interested in linguistics.

IL-43: Machine Learning-Driven Discovery of Pincer Complexes for Enhanced CO₂ Utilization

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Abstract

To advance catalyst development, understanding local reactivity is pivotal, dictated by the electrophilicity and nucleophilicity at active sites. Our previous research we performed extensive DFT study of various established a direct link between the electrophilicity of central metal atoms and catalyst performance, specifically turnover frequency (TOF) in carbon dioxide valorization.¹⁻⁴ However, performing condensed Fukui function calculations via DFT to evaluate electrophilicity of the central metal across numerous transition metal complexes is resource-intensive. Conversely, machine learning (ML) presents an appealing avenue to expedite catalyst discovery processes. The present study is not only accurate but also facilitates the examination of 285000 pincer complexes for their potential applications in CO₂ hydrogenation.⁵

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Dr. Vidya Avasare is a renowned educator and researcher in organic chemistry, serving as a faculty member since 1998 and currently heading the Department of Chemistry at SP College (2017–present). She earned her MSc in Organic Chemistry from Savitribai Phule Pune University (SPPU) and a Ph.D. in Organometallics from IIT Bombay. A recognized Ph.D. guide at SPPU, she mentors both MSc and Ph.D. students, fostering research excellence. Her contributions to academia include advancing PG organic chemistry courses and designing innovative programs like *Applied Organic Chemistry* as a Board of Studies member at SPPU (2017–2022). In 2021, she was honored with the prestigious *National Teacher Award* by the Indian National Science Academy, New Delhi. Dr. Vidya Avasare research focuses on sustainable catalysis, synthetic methodologies, and computational chemistry. Her work spans homogeneous and heterogeneous catalysis, CO₂ sequestration, N₂ activation, and hydrogen production, leveraging synthetic and machine-learning strategies. She has published extensively, including four cover-featured articles in ACS journals, and collaborates with industry partners on funded projects supported by CSIR, UGC, and DST-SERB.

IL-44: Catalytic Manipulation of Cellular Redox Processes for Enhanced Cancer Chemotherapy

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Abstract

Advances in cancer chemotherapy have traditionally focused on the stoichiometric use of drugs that interact directly with cellular targets in a 1:1 fashion. However, a new paradigm is emerging that leverages catalytic drugs capable of continuous turnover and redox cycling within cells, enabling sustained therapeutic effects at lower doses. This talk will explore the catalytic manipulation of cellular redox processes involving glutathione, NADPH, and reactive oxygen species (ROS) using rationally designed metal complexes.^[1,2,3] By selectively targeting cancer cell's dysregulated redox homeostasis, catalytic drugs (candidates) can induce oxidative stress beyond the cell's compensatory limits, leading to selective cancer cell death while sparing healthy tissues. I will discuss the design principles behind catalytic metallo-drugs, their mechanism of action, and their potential to overcome common challenges in chemotherapy, including drug resistance and toxicity. Case studies of platinum, iron, and rhenium-based agents will be presented to illustrate the practical application of this approach.

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IL-45: Multi-functional Core-shell Catalysts for Conversion of Carbon Dioxide

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Abstract

Core-shell structured catalysts, consisting of composite structures with one material partially or fully encapsulating another, offer the ability to combine complementary functionalities in controlled nanoscale geometries, making them highly tunable and ideal for applications in thermo-catalytic, photocatalytic, and electrocatalytic reactions. This talk will present two examples of the application of multi-functional properties of core-shell catalysts in CO₂ conversion reactions. In the first work, a novel sandwich structured Ni/SiO₂@CeO₂ catalyst, with Ni nanoparticles sandwiched between a siliceous core and a defect-rich CeO₂ shell, was used for thermo-catalytic Dry (CO₂) Reforming of Methane reaction. The core-shell catalyst showed exemplary stability and coke resistance in DRM, while achieving one of the highest reported turnover frequencies. Detailed characterization and mechanism studies suggest that the high activity and coke resistance of the core-shell catalyst can be attributed to a combination of physical obstruction of metal sintering and bifunctional catalysis by the abundant Ni/CeO₂ interfaces. *In situ* DRIFTS and TPSR-MS results evidenced the participation of lattice oxygen of CeO₂ in both CH₄ and CO₂ activation. In another example, the same catalyst with minor modifications was used for photothermal CO₂ hydrogenation to methane using simulated sunlight to enhance reaction rates. The core-shell catalyst demonstrated a 16-fold enhancement in product yields upon light irradiation at 250 °C and a 4-fold higher activity than corresponding supported metal catalysts. The role of the core-shell structure and Ni/CeO₂ interfaces in the enhanced photothermal activity was supported by *in situ* DRIFTS studies, FDTD simulations, and optical and chemical catalyst characterizations of the catalysts.

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Prof. Sonali Das's research interests lie in catalyst development for energy and environmental applications and in probing fundamental catalytic phenomena and reaction mechanism on well-defined catalysts. She earned her PhD from the National University of Singapore in Chemical Engineering, specializing in heterogeneous catalysis for carbon dioxide conversion, and a postdoc from UC Davis, working with Professor Bruce Gates on catalysis by metal organic frameworks and single atom catalysts. Prior to her PhD, she has a background in the oil and gas industry as a process engineer at UOP Honeywell for several years.

IL-46: Electrochemical Synthesis of N-based Products (Green Ammonia, Green Urea & Nitric Acid) Under Ambient Conditions: Fundamental and Translational Components

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Abstract

There are numerous varieties of fertilizers that primarily consist of macronutrients such as phosphorus, potassium, and nitrogen. Fixed nitrogen is often the limiting macronutrient for plant growth, making the production of nitrogen-based fertilizers—like ammonia, nitrate, and urea—a significant global challenge. To address the issue of global hunger over the next few decades, the use of nitrogen-based fertilizers is expected to rise. However, this increase will greatly impact energy consumption and the environment, as nearly all nitrogen-based fertilizers are produced using ammonia and nitric acid, both of which have high energy and carbon footprints. Therefore, it is essential to develop new technological solutions for producing ammonia, urea, and nitric acid without relying on fossil fuels.

In our laboratory, we have designed and developed electrocatalytic methods to produce green ammonia, green urea, and nitric acid under ambient conditions using specialized electrocatalysts. All of these processes are protected by appropriate intellectual property rights (IPR). We have successfully completed field trials for the synthesis of green ammonia and urea, and we have initiated the technology transfer and licensing process for pilot-scale production in collaboration with a multinational company.

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Dr. Uttam Kumar Ghorai is currently working as an Assistant Professor and Head of the Department in the Department of Industrial Chemistry and Applied Chemistry, Ramakrishna Mission Vidyamandira, Belur Math, India. Dr. Ghorai has made significant research contributions to the development of sustainable processes and products. The major emphasis of his research includes the synthesis of green ammonia, green urea, and nitric acid under ambient conditions using electrochemical pathways. He recently granted a license for the green ammonia synthesis process to multinational company with seven years of royalty terms for usage in the paint, coating, and textile sectors in India and abroad. Dr. Ghorai's contribution to electrocatalytic CO₂ capture and conversion to green urea technology aligns with the crucial contemporary challenge of carbon capture and utilization (CCU). Importantly, his process for utilizing CO₂ to produce green urea would address the issue of a sustainable environment while increasing agricultural output. The impact of his research is evident from the quality of publications he has in the last 5 years and the number of national/international recognitions he has received. Among various awards, a few awards need a special mention: Young Scientist Award from the Material Research Society of India- in 2018, Young Engineer Award from the Indian National Academy of Engineering (INAE) in 2019, and the Young Scientist Platinum Jubilee Award (in Chemical Sciences) from The National Academy of Sciences (NASI) in 2020. He is also the winner of the Merck Young Scientist Award 2023 in Chemical Sciences and recipient of the BRICS Young Innovator Prize 2022. He was elected as an Associate Fellow of the Indian Academy of Sciences (in 2021) and the Indian National Academy of Engineering (in 2019).

IL-47: Tuning the Physicochemical Attributes of Catalytically Active Materials for Better Understanding of Structure-Property-Performance Triad

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Abstract

Materials engineering has emerged as a holy grail for all modern-day challenges faced by human civilization. The realm and impact of efficient functional material design span drug delivery, electronic components, energetic materials, and climate change among others. However, the emission of GHG responsible for climate change is an existential threat that requires immediate attention. Some of the most explored solutions include the use of renewable sources of energy or photo/electrochemical reactions or CCUS technologies. These technological solutions require efficient catalytic material designs such as titania, and zeolites. The rational design of these crystalline products calls for a detailed understanding of mechanistic insights at the nanoscopic level. To this end, we will present our studies pertaining to titania and nanoporous zeolites to understand growth mechanisms and control physicochemical attributes such as shape, size, porosity, and elemental composition. Overall, the tuning of properties including, size¹, morphology², crystal planes³, Al speciation⁴, porosity speciation⁵, and Ti-site speciation⁶ have direct implications on the performance of these materials. Here, we will present our detailed studies on Anatase crystallization. Using suitable variation growth conditions and time-elapsing studies, we have developed the blueprint of growth pathways establishing the role of nanosheets, nanoparticles, and nanocrystallites to generate bulk crystals. These observations helped us generate the tapestry of particles varying in dimensionality (0D–3D), sizes (8–3000 nm), and morphology (aggregated to highly faceted crystals). These novel syntheses generated uniquely faceted particles with high-indexed surface planes such as (004), (200), and (105), amenable to photocatalytic applications. In a similar vein, we will present our studies on another class of inorganic materials, namely nanoporous zeolites, the ‘Golden Boy’ of the modern-day chemical industries. Keeping the diversity in consideration, we will present the pathways through which we were able to control Aluminum speciation in zeolite beta for better efficacy for phenol alkylation. The novelty of our approach was established using phenol alkylation with cyclohexanol wherein we observed the highest conversion and desired C-C alkylated product formation for the malonic acid-treated Zeolite Beta. Additionally, Octahedral titanium (TiO₆), recently identified in some frameworks, demonstrates enhanced catalytic activity, especially with larger reactant molecules, due to its distinct electronic and steric characteristics.⁸ To this end, we will present detailed studies for incorporating and tuning the Si/Ti ratio in small-pore zeolite SSZ-13 crystals. The incorporation of hierarchical mesopores into the framework results in lowering the effective diffusional path length thus increasing the selectivity, and catalyst lifespan⁹. Here, we will showcase innovative pathways for developing a single-pot method for generating core-shell faujasite which can be used as an efficient adsorbent. We will present comprehensive design principles for tuning the advanced functional materials amenable to desired performance.

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Prof. Manjesh Kumar research group is focused on developing the novel pathways for synthesizing advanced functional material to better understand the Structure-Property-Performance triad. In particular, our research interests lie in crystal engineering to tune the physicochemical attributes of nanoporous materials such as zeolite and MOF and metal/metal oxides such as titania. There are wide variety of targeted applications in catalysis and gas separation such as reverse water gas shift reaction, hydrocarbon cracking, CO₂ electrochemical reduction, methanol to olefins, alkylation, CO₂ capture, and H₂ separation among others. In order to obtain the efficient material, we delve deeper into the fundamental studies to develop growth mechanism which in turn help generate heuristics for crystal design.

Special Invited Speakers

SIL-1: *In situ/Operando* X-ray Absorption Spectroscopy for Energy Applications

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Abstract

In-situ/operando measurements during the course of a reaction involving energy materials like catalysis or charging/discharging process of a battery allow immediate observation of complex processes like volume fluctuations, phase transitions, change in oxidation state of the active species etc. and can detect non-equilibrium or short-lived intermediate species without any contamination/modification of samples which generally happen in case of *ex-situ* measurements. Synchrotron radiation based *in-situ/operando* X-ray Absorption Spectroscopy (XAS) measurement is extensively used for this purpose since XAS can probe a wide range of materials including nanomaterials, amorphous materials, polycrystalline materials, suspension in liquids, solution, aggregates etc. and can yield element specific information regarding geometric and electronic structure.

Over the last few years several facilities have been created at the EXAFS beamlines (BL-08 & BL-09) of the 2.5 GeV, Synchrotron Radiation Source (Indus-2) at RRCAT, Indore, India for carrying out *in-situ/operando* XAS measurements. This include facilities for (i) studying the initial stages of growth of nanoparticles from solution phase [1], (ii) probing the structural changes in catalysts during a catalysis/photo-catalysis or electro-catalysis reaction [2] and also (iii) for probing changes in electronic and geometric structures of electrode materials during the electrochemical reactions of rechargeable Li/Na ion batteries [3]. Various types of reactions cells have been custom-designed and fabricated in-house for these *in-situ/operando* XAS studies. This talk will present glimpses of all these facilities and will also elaborately describe the results of few operando experiments [4-6].

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Dr. Chandrani Nayak is currently scientist at Atomic and Molecular Physics Division, Bhabha Atomic Research Centre, Mumbai, India. She is involved in characterization of many technological important samples by Synchrotron based X ray Absorption Spectroscopy using the EXAFS facility at Indus 2, RRCAT, Indore. Her main research interest is studying the structural changes around metal cations during various processes like growth of nanoparticles, heterogenous catalytic reactions, photocatalytic reactions, electrochemical reactions, charging-discharging of batteries, etc. using *in situ/operando* time resolved XAFS. She is recipient of Young Applied Scientist Award of Department of Atomic Energy, Govt. of India in 2020 for *In- situ/operando* studies using Synchrotron radiation based X-ray absorption Spectroscopy.

SIL-2: Temperature-Dependent Tunnelling Mechanisms in Intersystem Crossing Pathways of Carbenes

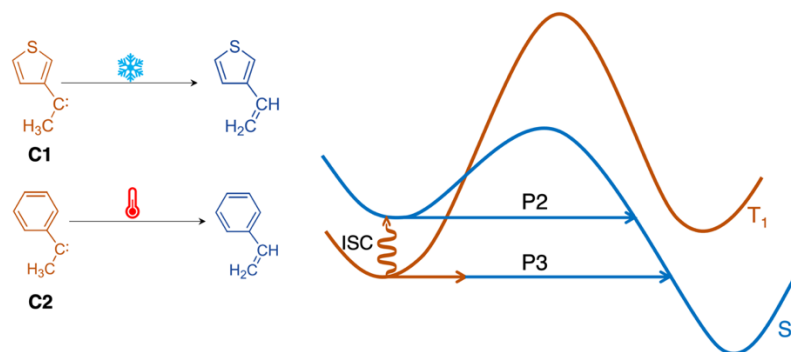
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Abstract

Matrix-isolation experiments at cryogenic temperatures uncovered tunnelling in the intersystem crossing (ISC) pathways of two carbenes: 1-(3-thienyl)-ethylidene (**C1**) and 1-phenylethylidene (**C2**) from their excited triplet (T_1) to ground singlet state (S_0).¹ While tunnelling was observed in **C1** at 10 K, **C2** needed to be heated to 65 K, pointing to temperature-dependent mechanisms. In this work, we have used an instanton formulation of Fermi's golden rule²⁻³ to uncover these reaction mechanisms. Instanton theory treats molecules in full dimensionality using *ab initio* potential energy surfaces, thus allowing us to leverage accurate multireference calculations. We find three possible pathways exist for the ISC mechanism: P1 involves tunneling on T_1 followed by ISC to S_0 , and is ruled out due to a high barrier on T_1 ; P2 starts with ISC up to S_0 , followed by tunnelling through a barrier on S_0 , and this channel is available at higher temperatures; P3 is the most interesting of all and involves a change in electronic character along the H-transfer tunnelling pathway.⁴ P3 has a near constant rate across temperatures and is responsible for the tunnelling observed in **C1**. In **C2** tunnelling can only take place through P2 at higher temperatures. This work describes a novel ISC mechanism which involves switching of electronic states while tunnelling through a barrier.



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Meghna A. Manae obtained her PhD in Indian Institute of Science Education and Research (IISER) Pune under the supervision of Anirban Hazra in December 2019, specializing in electronic structure of excited states. This was followed by a postdoc (2020-2021) in Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR) in the group of Umesh V. Waghmare, studying computational heterogeneous catalysis. Currently, she is a postdoc at ETH Zürich in the group of Jeremy O. Richardson, working on reaction rates and mechanisms using instanton theory, with a particular interest in nonadiabatic reactions.

SIL-3: Plasmon-Enhanced Solar Powered “Hot Electron” Catalysis in Black Gold-Nickel

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Abstract

Conventional plasmonic nanocatalysts have intense light absorptions but are narrow.^{1,2} In this work, we have designed and synthesized dendritic plasmonic colloidosomes of Au (black gold)³, based “antenna reactor” of nickel that absorbs across the entire optical range.^{4,5} The plasmon-induced hot electrons and the intense electric field within the hotspots of black gold interact with reactants adsorbed on the Ni sites to activate the chemical bond. Black Gold-Ni exhibited exceptional performance in photocatalytic CO₂ hydrogenation, achieving a CO production rate of $2464 \pm 40 \text{ mmol g}_{\text{Ni}}^{-1} \text{ h}^{-1}$ with 95 % selectivity and was stable for over 100 h. The photocatalytic reaction showed a superlinear power law dependence on light intensity, and a higher kinetic isotope effect in light than that in the dark, affirming a hot-electron-mediated mechanism. Operando DRIFTS confirmed that CO₂ hydrogenation takes place via a direct dissociation pathway through linearly bonded Ni–CO intermediates.⁴ Additionally, the black gold-Ni catalyst was effective in catalyzing other challenging reactions like hydrodechlorination of dichloromethane and hydrogenation reactions.⁵ These findings suggest that the black gold-Ni “antenna-reactor” system holds significant potential for advancing plasmonic catalysis, particularly in the strategic reduction of CO₂ and other energy-intensive reactions under mild conditions using solar energy.

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Mr. Rishi Verma is a research scholar in the Department of Chemical Sciences, TIFR, Mumbai. He holds a Bachelor's degree in chemistry from Ramjas College, University of Delhi (2018). He then joined the Nanocatalysis lab in the Department of Chemical Sciences, TIFR, Mumbai as an integrated Ph.D. student. For his master's thesis, he explored the impact of defects or oxygen vacancy on the acidity of Amorphous Aluminosilicates. During his doctoral work, he worked on the development of a photocatalyst to carry out challenging reactions using light. His research focuses on plasmonic systems, based on plasmonic black gold for photocatalytic CO₂ hydrogenation, hydrodechlorination, and hydrogenation reactions. He has presented his research at over 22 international and national conferences. He won the first prize in the new generation ideation contest (NGIC)-2021 at HP Green R&D Centre, Bengaluru, India. He also received the Best Poster Award in the Energy and Materials theme at the 3rd Commonwealth Chemistry Posters 2022 and has won multiple Best Poster and Oral Presentation awards at various conferences.

SIL-4: Probing Photophysical and Photochemical Processes in a Nanoscale Gap

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Abstract

Light-matter interaction plays a vital role in energy conversion and storage-related problems in modern society. The absorption or emission of light typically occurs on the sub-nanometer scale. Hence, delving into the fundamental aspects of light-matter interaction through atomic-scale exploration becomes profoundly significant. Among various conceivable methods, the utilization of localized surface plasmons (LSPs) stands out as a remarkably appealing and effective strategy for amplifying light-matter interaction.^[1] In simpler terms, LSPs entail the collective oscillation of free electrons within noble metal nanostructures (Ag or Au), resonating with the electric field of incident light.

On the other hand, a scanning tunneling microscope (STM) serves to visualize surfaces at the atomic scale by means of quantum tunneling. Consequently, the interaction between light and matter on atomic scales can be investigated by combining light with an atomically sharp, plasmonically active STM tip. Light confinement in this manner significantly enhances the usually faint Raman scattering signal from a single molecule by multiple orders of magnitude, a method referred to as tip-enhanced Raman spectroscopy (TERS).^[2] Moreover, the confined light can also trigger the activation of certain chemical bonds, identified as plasmon-mediated chemical reactions (PMCRs). This talk sheds light on the comprehensive exploration of TERS and PMCRs, encompassing a diverse array of real-life applications.^[3-5]

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SIL-5: Pincer-Type Palladium Sites in an Asymmetrical Covalent Organic Framework as a Single-Atom Catalyst for Miyaura Borylation and Self-Cascade Coupling

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Abstract

Efficient and well-defined support materials are crucial for stabilizing single-atom catalysts (SACs), preventing agglomeration, and optimizing atom efficiency.¹ They fine-tune electronic properties and reaction environments, boosting stability, activity, and selectivity in catalytic processes.²

In this study, we report the synthesis of a novel covalent organic framework (COF) featuring spherical morphology and functional pincer-type ligands for the stabilization of palladium (Pd) SACs. This innovative material demonstrated remarkable catalytic activity and selectivity in the Miyaura borylation of aryl halides with diboranes under mild conditions.³ Additionally, the catalyst enabled efficient in-situ borylation followed by highly selective homo- and hetero-Suzuki coupling reactions, delivering excellent yields.⁴

Mechanistic investigations, supported by computational calculations, revealed the importance of the active sites and base in achieving selective borylation. The Pd-SAC exhibited exceptional stability and recyclability, underscoring its potential for sustainable, scalable catalytic processes.

Furthermore, we developed a Pd single-atom catalyst stabilized on graphitic carbon nitride (gC₃N₄), which was applied to the stereoselective Heck coupling of challenging substrates with high success.⁵ This work highlights the versatility and promise of Pd SACs supported by COF and gC₃N₄ in advanced catalytic applications.

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Dr. Vitthal Saptal's research lies at the forefront of advanced catalyst design and sustainable chemical transformations. His expertise encompasses the development of both homogeneous and heterogeneous catalysts for challenging organic reactions and the conversion of carbon dioxide into valuable chemicals and fuels through environmentally sustainable processes.

A core focus of his work is designing tailored coordination environments for the efficient stabilization of single-atom catalysts (SACs), significantly enhancing their activity and selectivity. His research also delves into innovative strategies for transforming complex organic substrates into value-added products.

Dr. Saptal earned his Ph.D. in 2019 from the Institute of Chemical Technology, Mumbai, India. He has gained extensive international research experience through stints in South Korea, China, Poland, and Italy. In 2022, he was awarded the prestigious Marie Skłodowska-Curie Actions (MSCA) fellowship at Politecnico di Milano, Italy, with the highest evaluation score for his postdoctoral research. His academic achievements are further highlighted by the Institute Postdoctoral Fellowship (IPDF) from the Indian Institute of Technology Kanpur (IITK) and the Eklavya Scholarship.

SIL-6: Multicomponent Covalent Organic Frameworks: Design to Function

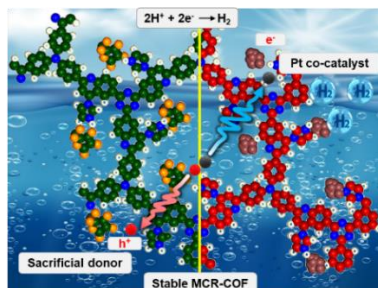
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Abstract

In nature, organic molecules play a vital role in light harvesting and photosynthesis. However, regarding artificial water splitting, research is primarily focused on inorganic semiconductors. Although organic photocatalysts, such as recently developed covalent organic frameworks (COFs), have high structural variability, they tend to exhibit lower quantum efficiencies for water splitting than their inorganic counterparts.¹ A **multicomponent** reaction (MCR) involves at least three or more components that combine in a cascade manner to provide a single product in a one-pot synthesis.² The use of MCRs to build COFs seems to be an excellent way to create COFs with high stability. We have recently presented the synthesis of various new multifunctional microporous MCR-COFs via irreversible three-components Doebner, Povarov and Domino reaction.³⁻⁵ This presentation will highlight the fundamental importance of functionalized pores within the COF skeleton for understanding its properties and performance, particularly in photocatalysis. Additionally, this presentation will discuss various MCRs employed in the synthesis of novel COFs and address critical challenges associated with achieving stable and long-term photocatalytic water splitting.



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Dr. Prasenjit Das received a B.Sc. (Hons.) degree from the University of Calcutta in 2011, and an M.Sc. degree in Chemistry from IIT Hyderabad, India in 2013. He received his Ph.D. degree from IISER Mohali, India, under the supervision of Prof. Sanjay K. Mandal in May 2019. His Ph.D. work focussed on the design of functional MOFs and COFs for energy and environmental applications. In November 2019, he received prestigious Alexander von Humboldt postdoctoral fellowship from Humboldt foundation. He did his first postdoctoral research under the supervision of Prof. Nathaniel L. Rosi at the University of Pittsburgh, USA from 2019-2021. His postdoc work focussed on the design of stratified NIR-MOFs for bioimaging. In November 2021, he joined as a Alexander von Humboldt postdoctoral fellow for pursuing postdoctoral research under the supervision of Prof. Arne Thomas, TU Berlin, Germany. His current research work is focussed on Pore functional COFs for solar to chemical energy conversion.

SIL-7: Harnessing Electrochemical Power to Convert CO₂ into C₄ Oxyhydrocarbon and Polymer

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Abstract

The electrocatalytic conversion of CO₂ to multi-carbon products offers a promising route for carbon capture and conversion. While significant progress has been made in improving the efficiency and selectivity of CO₂ reduction reactions (CO₂RR), challenges remain, particularly in achieving high Faradaic efficiencies (FE) for higher molecular weight products (C_n, n > 2).¹⁻³ This study focuses on the performance of CuP₂, a transition metal phosphide, as an electrocatalyst for CO₂RR. CuP₂ was synthesized using a hydrothermal method, yielding a porous, phase-pure material. Electrochemical testing revealed that CuP₂ catalyzed the production of formic acid, methylglyoxal, and 2,3-furandiol, with 2,3-furandiol as the dominant liquid product.⁴ The FE for C₄ product reached 36%, with an overall FE of 44% at -0.6 V vs. RHE. Notably, CuP₂ required a higher overpotential compared to other metal phosphides like Ni₂P, with an overpotential of -1.9 V vs. RHE to reach -10 mA/cm², which could be attributed to its semiconducting nature.^{5,6} A distinct feature of this catalyst was the formation of a polycarbonate polymer via esterification reactions at higher currents. Despite the large overpotential, CuP₂ showed stability under longer testings, demonstrating its potential for CO₂ utilization. These findings contribute to the understanding of transition metal phosphides in CO₂ electroreduction and highlight CuP₂'s potential for generating valuable multi-carbon products.

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Dr. Mahak Dhiman got his PhD in Chemistry from TIFR-Mumbai, working in Prof. Vivek Polshettiwar's group. His research involved developing advanced catalysts, including pseudo-single atom Pt and Au on DFNS and gold plasmonic colloidosomes. He further refined his expertise during the postdoctoral work at Rutgers University, where he specialized in electrocatalysis for converting CO₂ into fuels. Currently, at CSIR-IIP, his focus is on advancing CO₂ conversion technologies to produce sustainable aviation fuels (SAF). His research focuses on catalysis, electrochemistry, and photochemistry to address sustainable energy and environmental challenges. He specializes in CO₂ conversion into fuels and chemicals via electrochemical and photochemical pathways. His contributions include work on electrocatalytic CO₂ reduction to C₃ and C₄ chemicals and promoting the Power-to-Liquid (PtL) pathway for sustainable aviation fuels.

Poster List

Poster No.	Name	Institute	Abstract Title
CI P-01	Shibani Mohata	Indian Institute of Science Education and Research, Kolkata	Selective Metal-Free CO ₂ Photoreduction in Water Using Porous Nanostructures with Internal Molecular Free Volume
CI P-02	Vipin Kamboj	Indian Institute of Science, Bangalore	Solid Oxide-Based Electrodes for CO ₂ Reduction
CI P-03	Satyam Gupta	Indian Institute of Technology, Kanpur	Flue Gas Reforming of Methane using Ni-Al ₂ O ₃ and Ni-Co-Al ₂ O ₃ Catalysts
CI P-04	Ravi Kumar	Indian Institute of Science Education and Research, Bhopal	Exploring Bis-NHC Amino Pincer Ligand-Based Bifunctional Ru and Mn Complexes toward Catalytic Hydrogenation of CO ₂
CI P-05	Saroj Kumari	Indian Institute of Technology, Kharagpur	A DFT Study of Biomimetic CO ₂ Hydration Reaction on High-Index Ni (211) Surface
CI P-06	C D Balaji	Indian Institute of Technology, Madras	Mechanistic Investigation for CO ₂ Hydrogenation to Methanol and Methanol Conversion to Hydrocarbons
CI P-07	Amitabha Das	Indian Institute of Technology, Indore	DFT and ML Methods for Screening of Homogeneous/Heterogeneous Catalysts for C1/C2 Products from CO ₂
CI P-08	Shreya Singh	Indian Institute of Technology, Delhi	Optimizing Heterogeneous Photocatalyst Design for CO ₂ Reduction to Fuels
CI P-09	Ayaj Ansari	Indian Institute of Technology, Kanpur	Hydrate Formation in the Presence of Promoters for CO ₂ Capture and Storage Application
CI P-10	Vaishnavi Kulkarni	Indian Institute of Technology, Indore	Synthesis and Characterization of Adsorbents for Direct Air CO ₂ Capture
CI P-11	Ritu Bharadwaj	Indian Institute of Science Education and Research, Bhopal	Integrated CO ₂ Capture and Conversion: Probing NHC-Based Organometallic Catalysts
P-001	B. Sathya Sai Rengam	Indian Institute of Technology, Madras	Elucidation of the Mechanisms Behind Selective Oxidation of Methane to C1 and C2 Oxygenates Over FeAu/ γ -Al ₂ O ₃ Catalysts
P-002	Vasudha Sharma	Indian Institute of Technology, Bombay	Carbon dioxide Transformation to Sustainable Energy and Fuels using Low coordinated Molecular Catalyst
P-003	Sunil Kumar Sahoo	Indian Institute of Technology, Kharagpur	Thermocatalytic CO ₂ Utilization by Oxidative Dehydrogenation of Propane using Mixed Metal Oxides: An Alternative Approach to CrO _x Based Catalysts
P-004	Saurabh Kumar	Indian Institute of Science Education and Research, Bhopal	CO ₂ Hydrogenation to Formate by Molecular Ir Complex-Based Polymeric Catalyst
P-005	Rushikesh Khilari	CSIR- National Chemical Laboratory, Pune	Kinetic and Mechanistic Study of Structured Catalyst for Dry Reforming of Methane Reaction
P-006	Jyoti Tekawadia	CSIR-National Chemical Laboratory, Pune	Molybdenum Carbides: An Alternative Route for Methanol Synthesis by CO ₂ Hydrogenation and its Mechanistic Insights
P-007	Hushan Chand	Politecnico di Milano, Milan	A Zinc Single-Atom Catalyst for Efficient CO ₂ Fixation into Cyclic Carbonates
P-008	Sairam S	Indian Institute of Technology, Madras	Structure, Activity and Reaction Pathway of Ni-Ru/ γ -Al ₂ O ₃ Catalysts for CO ₂ Methanation
P-009	Kapil Bhati	CSIR- Indian Institute of Petroleum, Dehradun	Ni/Ce _{0.8} Zr _{0.2} O ₂ Solid Solution Catalyst: A Pathway to Coke-Resistant CO ₂ Reforming of Methane
P-010	Vasanthmani I	Pondicherry University, Pondicherry	Effect of KOH Activation on the CO ₂ Adsorption-Desorption Potential in Agro-Waste Biomass
P-011	Siddhartha Pandya	Guru Nanak Khalsa College of Arts, Science & Commerce, Mumbai	Structural Insights into CO ₂ Reduction by Formylmethanofuran Dehydrogenase
P-012	Hanumant Balaso Kale	Institute of Chemical Technology, Jalna	Nitrogen-enriched Mesoporous Carbon Nitride (C ₃ N ₅) for Chemical CO ₂ Fixation
P-013	Gaurav Vishwakarma	National University of Singapore	Dry Water CO ₂ Hydrates for Carbon Capture and Storage
P-014	Atmaja Shinde	Birla Institute of Technology and Science Pilani, Hyderabad	Synergistic Catalysts for CO ₂ Methanation: Synthesis, Characterization, and Mechanistic Studies of Co/NiO-MgO Nanocomposite
P-015	Aritra Guha	Indian Institute of Technology, Bombay	Visible light Driven Selective Production of Formate from CO ₂ by Homogeneous Co-Based Molecular Catalysts in Presence of Different Additives
P-016	Lavanya Yalagandula	Birla Institute of Technology and Science Pilani, Hyderabad	Dual-functional Catalyst for Efficient CO ₂ Conversion into Value-added Products
P-017	Deepanjan Patra	Indian Institute of Science Education and Research, Kolkata	Bismuth Incorporated g-C ₃ N ₄ as an Efficient Catalyst for Light-assisted CO ₂ Fixation at Room Temperature under Atmospheric Pressure
P-018	Mukesh Kumar	Indian Institute of Technology, Gandhinagar	Natural Kaolin Derived Ruthenium Supported Nanoporous Geopolymer: A Sustainable Catalyst for CO ₂ Methanation

P-019	Sneha Raj V. P.	Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore	Heterostructure Nanocatalyst based on Ce-MOF and MoS ₂ Towards Visible Light Driven CO ₂ Reduction to Ethanol
P-020	Suman Maity	Indian Institute of Technology, Bombay	Photocatalytic CO ₂ Reduction Using Mononuclear Self-Photosensitized Ruthenium Complexes: Utilization of Blue, Green, and Red Light
P-021	Huldah Suharika Chitturi	Birla Institute of Technology and Science Pilani, Hyderabad	Exploring the Significance of CO ₂ Methanation Studies on Co ₃ O ₄ and Ni-doped Co ₃ O ₄ Catalysts
P-022	Jaffar Ali B. M.	Pondicherry University, Pondicherry	Tailoring 2D Ti ₂ CT _x MXenes Photocatalytic Systems for CO ₂ reduction: Quest for Selective Ethanol Production
P-023	Deeksha S	Indian Institute of Technology, Madras	A Novel Method to Assess Amine Solvent Degradation & Corrosivity in Post-Combustion CO ₂ Capture Systems
P-024	Abhimanyu Singh Khichi	Indian Institute of Technology, Madras	Experimental Investigation of CO ₂ Absorption and Desorption Performance using Blended Amine Solvents
P-025	Pavan Kumar Kunigiri	Indian Institute of Technology, Dhanbad	“CO ₂ Activation, Utilization Using Mixed Metal Oxides” and Kinetic Study of Methanol Synthesis
P-026	Shunmuga Sundaram Shanmugam	CSIR - Central Electrochemical Research Institute, Karaikudi	Electrodeposited Bimetallic Copper Based Alloys as Electrocatalysts for CO ₂ Reduction
P-027	Biplop Jyoti Hazarika	Indian Institute of Science Education and Research, Kolkata	Efficient Halogen-Free Bifunctional Organocatalyst for CO ₂ Fixation into Cyclic Carbonates
P-028	Shivangi Singh	Indian Institute of Technology, Delhi	Electrochemical Work Function Modulation of SrTiO ₃ /Ti ₃ C ₂ T _x Heterostructure Towards Enhanced CO ₂ Reduction to Methane
P-029	Aathira B	Birla Institute of Technology and Science Pilani, Hyderabad	Engineering Defects for Enhanced Catalytic Dry Reforming of Methane
P-030	Dhiraj Ingle	Indian Institute of Technology, Hyderabad	Post-Synthetic Imidation of Conjugated Porous Polymers: Enhanced CO ₂ Capture And Selectivity
P-031	Adithyan P	National Institute of Science Education and Research, Bhubaneswar	Terahertz Conductivity of Free-Standing 3D Covalent Organic Framework Membranes Fabricated via Triple-Layer-Dual Interfacial Approach
P-032	Litty Sheji C	CSIR-National Chemical Laboratory, Pune	Biopolymeric Composite Membrane Blend with Mobile Carrier for CO ₂ /Gas Separation
P-033	Abhik Manna	Indian Institute of Technology, Bombay	Copper-Based Multi-Metallic Catalyst for Electrochemical Carbon Dioxide Reduction
P-034	Anjali Devang	CSIR-National Chemical Laboratory, Pune	Fabrication of Porous Support on Non-Woven Fabric for CO ₂ Separation Applications
P-035	Jitendra Kumar Prabhakar	Indian Institute of Technology, Kanpur	Metal Loading Effect and Comparative Analysis of Supported Monometallic Rh, Ni and Bimetallic Ni-Fe Catalysts for Efficient CO ₂ Methanation
P-036	Vanshree Parey	Harish-Chandra Research Institute (HRI), Allahabad	Strain-Engineered Bismuth Oxysulfide (Bi ₂ SO ₃) for Enhanced Electro- and Photocatalytic Performance in Water Splitting and CO ₂ Reduction
P-037	Suraj Kumar	Indian Institute of Technology, Madras	Unlocking CO ₂ Hydrate Kinetics: Amino Acid Promoters in Industrial-Scale CCS
P-038	Nikitra Gupta	CSIR-National Chemical Laboratory, Pune	Novel, Synergistic Oxide Catalysts: Transforming CO ₂ into Carbonate(s)
P-039	Eti Pagar	Indian Institute of Technology, Roorkee	Enhancing CO ₂ Hydrate Formation Kinetics in Saline Conditions Using Biodegradable Additive for CO ₂ Sequestration
P-040	Akhil Chandran P	Birla Institute of Technology and Science Pilani, Hyderabad	Post Synthetic Exchange in Zirconium Metal-Organic Framework for Efficient Photoreduction of CO ₂ to Formate.
P-041	Soniya Varghese	Indian Institute of Technology, Madras	Electrochemical co-Reduction of CO ₂ and Nitrate to Urea
P-042	Soham Raychowdhury	Indian Institute of Science, Bangalore	CO ₂ Electroreduction in CeO ₂ : Role of Doping on Oxygen Defect Formation using DFT+U Studies
P-043	Chinmay Girigosavi	CSIR-National Chemical Laboratory, Pune	Methane Pyrolysis: Advancing Towards Green Hydrogen Production
P-044	Amarnath T. M.	The Bombay Textile Research Association, Mumbai	Atmospheric Plasma Assisted Graphene Coating for Enhanced Properties of Polypropylene Fabric
P-045	Santosh Srinivas	Sastra Deemed University, Thanjavur	Photoreductive Dechlorination of Chlorpyrifos using 1D Poly(Heptazine imide) Photocatalysis
P-046	Shreya Tyagi	Indian Institute of Science Education and Research, Pune	Harnessing Light-Matter Interactions with Plasmonic Copper Nanoparticles for Photothermal Studies
P-047	Adhra Sury	Indian Institute of Science Education and Research, Pune	Enabling Photocatalysis Beyond the Redox Potential of Quantum Dots
P-048	Uttam Sharma	Indian Institute of Technology, Bombay	Plasmonic Ag@Cu Bimetallic Nanostructure for Hot Electron Induced CO ₂ Reduction at Room Temperature

P-049	Gangadhar Mahar	National Institute of Technology, Warangal	Agro-industry Waste Derived Akermanite Nanoparticles as Photo Catalyst for Industrial Waste Water Purification
P-050	Manoj Singh	Indian Institute of Technology, Gandhinagar	Highly Efficient Photocatalytic Hydrogen Generation Using Water-Stable Low-Dimensional Metal Halide Perovskites
P-051	Sri Himaja Pamu	Birla Institute of Technology and Science Pilani, Hyderabad	Enhancement of Visible Light Photocatalytic Activity of g-C ₃ N ₄ by tuning Bandgap and Morphology
P-052	Rahul Gaikwad	Institute Of Chemical Technology Mumbai, Jalna	Bimetallic Copper and Zinc Single-Atoms Decorated on Graphitic Carbon Nitride for Photocatalytic Carbon Dioxide Reduction to Methanol
P-053	Akash Bisoyi	Indian Institute of Science Education and Research, Thiruvananthapuram	α -C(sp ³) -H (Hetero)Arylation of Thioethers Enabled by Photoexcited Triplet Ketone Catalysis
P-054	Anish Kumar Mazumdar	Indian Institute of Technology, Kharagpur	Photocatalytic Nitrogen Fixation of Oxygen Vacancy Enabled Pd-TiO ₂
P-055	Srayee Mandal	Indian Institute of Science Education and Research, Berhampur	Emergence of Sustainable Sulfur Nanomaterials for Efficient Solar to Energy Conversion
P-056	Nur Jalal Mondal	Institute of Advanced Study in Science and Technology, Guwahati	Au-MoS ₂ Quantum Dot Composites: Structural Modification for Enhanced Catalytic Efficiency in p-Nitrophenol Reduction
P-057	Ripan Mondal	Indian Institute of Technology, Kharagpur	Ag NPs modified Ag ₂ AsO ₄ /g-C ₃ N ₄ Hybrid for Effective Photocatalytic Removal of 4-Chlorophenol Under Visible Light
P-058	Yeddula Nikhileshwar Reddy	Center of Innovative and Applied Bioprocessing, Mohali	Metalloporphyrin based Solar Photocatalytic Degradation of Lignin
P-059	Emmanuel Kunnel	Indian Institute of Technology, Kharagpur	Selenium-Loaded Bi ₂ WO ₆ /g-C ₃ N ₄ Hydrogels for Tetracycline Degradation with Visible Light-Activated Peroxymonosulfate
P-060	Bitopan Boro	Institute of Advanced Study in Science and Technology, Guwahati	Self-Assembly of Plasmonic Nanoparticles upon Interaction with Amino Acids
P-061	Maheswari Yadav	Indian Institute of Technology BHU, Varanasi	At Circumneutral pH Photocatalytic Activity of p-Nitrophenol by Starch Composite Mo Doped Iron Pyrite Nanoparticles
P-062	Sudhanshu Pandey	Pondicherry University, Pondicherry	Photocatalytic Water Splitting by WO _{3-x} /g-C ₃ N ₄ Heterostructure Nanocomposites for Green Hydrogen Production
P-063	Varsha Kare	Institute of Chemical Technology, Mumbai	Effect of Aqueous DES as Reaction Media for Photocatalysed Amine Oxidation
P-064	Rituraj Borah	University of Antwerp, Belgium	Nanoscale Energy Balance of Plasmonic Antenna-Reactor Catalyst for Light Driven Reactions: Role of Hot Carriers vs. Photothermal Effect
P-065	Vishwas Saini	CSIR-Indian Institute of Petroleum, Dehradun	Nanomaterials and Biomass-Based Composite Membrane for Water Treatment Application
P-066	Swadhin Kumar Jena	Indian Institute of Technology, Mandi	Metal Organic Frameworks Decorated Polypyrrole Nanorod as Super-Adsorbent Towards Pollutants in Continuous Flow
P-067	Nikita Rao	Indian Institute of Science, Bangalore	Carbon Sequestration and Structural Changes in Soil-Based Alkali Activated Binders
P-068	Manisha Sharma	Indian Institute of Technology, (BHU), Varanasi, India	Multicomponent Heterojunction Photocatalyst NGT/g-C ₃ N ₄ /BiOBr _{0.75} I _{0.25} for UV-Visible-NIR Responsive Photocatalytic Degradation of Rhodamine B
P-069	Shabnam Dan	Sam Higginbottom University of Agriculture, Technology and Sciences, Prayagraj	Simultaneous Degradation of Cr (VI) and Methylene Blue by PEG Modified Manganese Ferrite (MnFe ₂ O ₄): Nanoadsorbent and Photocatalyst
P-070	Krishnarao Desai	Vellore Institute of Technology, Vellore	Blue-LED-Driven Green Chemistry: Pioneering Sustainable Strategies for C-X Bond Formation
P-071	Anusha Jain	Indian Institute of Technology, Delhi	The Magic of Morphology: A TiO ₂ Story
P-072	Suman Das	Indian Institute of Technology, Mandi	One-Pot Photoreforming of Polylactic Acid Waste to Valuable Chemicals
P-073	Shreya Sarkar	Birla Institute of Technology and Science Pilani, Hyderabad	Investigating plasmonic catalysis of C-C/C-N Coupling Reactions in Water using bi-metallic Ag-Cu/Ag-Co substrates via in-situ SERS
P-074	Akanksha Sharma	Indian Institute of Technology, Gandhinagar	Plasmon-mediated Green Hydrogen from Organosilane Waste Under Sunlight with Value-Added Co-Products
P-075	Murthy Dharmapura	Manipal Institute of Technology, Manipal	Ir ³⁺ or Ir ⁴⁺ : Intriguing Role of Ir Valence State on the Photocatalytic H ₂ Generation in Visible-Light Absorbing Ir-Doped BaTiO ₃
P-076	Chitara Rajeshkumar	St. Xaviers College, Ahmedabad	Efficient Photocatalytic CO ₂ Reduction of the AsXBr (X= S, Se and Te) Heterostructures
P-077	Simon Joyson Galbao	Manipal Institute of Technology, Manipal	Intriguing role of N-vacancies and p-states in Extending the Optical Absorption and Photocatalytic H ₂ Evolution in Copolymerized g-C ₃ N ₄
P-078	Bhagyalakshmi Chinnam	National Institute of Technology, Warangal	Investigating the Effect of Various Process Parameters on Visible Light-Driven TiO ₂ -based Photocatalysis for the Remediation of Aqueous Phase Polystyrene Microplastics

P-079	Suchashrita Mitra	Birla Institute of Technology and Science, Hyderabad	Fluorinated Transition Metal-based MOF with Enhanced Water Stability for Efficient CO ₂ Reduction
P-080	Alisha Sengupta	Ashoka University, Sonapat	Diphenylanthracene-based Trimeric Systems for Efficient Photon Upconversion through Triplet-Triplet Annihilation
P-081	Jeebanjyoti Mohapatra	National Institute of Science Education and Research, Bhubaneswar	Construction of Imine-linked Nanoparticle Organic Networks for Field Effect Transistors
P-082	Bhagyashree Priyadarshini Mishra	Indian Institute of Technology, Mandi	Sr-doped MoO ₃ for Photocatalytic N ₂ fixation
P-083	Astha Tyagi	Indian Institute of Science, Bangalore	Thermally Stable Li ⁺ co-doped ZnMoO ₄ : Eu ³⁺ Phosphors for White LED Applications and Selective Sensing of Nitroaromatic Compounds
P-084	Shamim Hossain Shah	Indian Institute of Technology, Guwahati	Halide-Dependent Regulation of Energy and Electron Transfer in CuInS ₂ -Decorated Perovskite Nano-heterostructure
P-085	Femina Cherumannil	Farook College, Kozhikode	Structural and Theoretical Investigation of Photophysical Properties In Anthracene-Cyanostilbene Based Donor-Acceptor Systems
P-086	Shukla Majhi	Banaras Hindu University, Varanasi	Construction of Inverse Vulcanized Sulfur Polymer embellished with Silver Nanoparticles for SERS Screening of Hazardous Colorants and Antibiotic in Contaminated Water
P-087	Nikita Braganza	Institute Of Chemical Technology, Mumbai	Spectroscopic Evidence of Improper H-bonds Formed in Alkanolamines Used in CO ₂ Capture
P-088	Santanu Dolai	Indian Institute of Technology, Guwahati	Influence of Dimensionality on Optical Properties of Doped Assembly of Gold Nanoclusters
P-089	Kamali Kesavan	CSIR-Institute of Minerals and Materials Technology, Bhubaneswar	High-Pressure SERS Effect on ZIF-67/R6G System
P-090	Arif Khan	Indian Institute of Technology, Roorkee	Synthesis of Kraft Lignin-Based Conductive Resin and its Application in Sensor and Flexible Electronics
P-091	Arti Saroj	Indian Institute of Technology-BHU, Varanasi	pH Dependent Study of Isatin Based Drugs Using Raman Spectroscopy and SERS
P-092	Sankaran Ramesh	Lund University, Sweden	Coherent Phonons and Charge Carrier Localization in Cesium Gold Bromide
P-093	Rashi	Institute of Nanoscience and Technology, Mohali	Probing the Fluorescence Intermittency of Bimetallic Nanoclusters using Single-Molecule Fluorescence Spectroscopy
P-094	Zahir Abbas	Indian Institute of Technology, Indore	Triboelectric Nanogenerators Enhanced by a Metal-Organic Framework for Sustainable Power Generation and Air Mouse Technology
P-095	Chandan Kumar	Nagoya University, Nagoya	Aggregation and Crystallization Studies of DNA Functionalized Nanoparticle for Enhanced Optical Response
P-096	Amit Kumar	Indian Institute of Science Education and Research, Mohali	Room-Temperature Polaron Dynamics in Lead-free Cs ₄ CuSb ₂ Cl ₁₂ Layered Double Perovskite Nanocrystals
P-097	Shashi Gomi	Tata Institute of Fundamental Research, Mumbai	Forcing Isomerization Pathways to Completion inside Water-soluble Nanocages
P-098	Komal Thawrani	Tata Institute of Fundamental Research, Mumbai	Photocatalytic H ₂ O ₂ Production by Heptazine Hydrazine Polymer
P-099	Rajesh Bera	The Institute of Photonic Sciences, Barcelona	Mid-Infrared Active Non Toxic Colloidal Quantum Dots
P-100	Debasish Barman	Kyushu University, Japan	Triplet Harvesting TADF Emitters Towards Energy-Efficient Organic Electronics
P-101	Charvi Singhvi	Tata Institute of Fundamental Research, Mumbai	Designing Electronically Tuned Defect-Rich Trimetallic-Ceria Catalytic Sites for Enhanced CO ₂ Reduction Reaction
P-102	Swayamprakash Biswal	Indian Institute of Technology, Delhi	Single Atom Induced Ferromagnetism for Magneto-electrocatalytic Water Splitting Reaction
P-103	Komalpreet Kaur	Indian Institute of Science Education and Research, Mohali	Ultrathin-Highly Twisted PdNi Alloyed Nanowires for High-Performance Fuel Cell Reactions
P-104	Jithul K. P.	Birla Institute of Technology and Science, Pilani	Development of Manganese-Nitrogen-Carbon Bifunctional Electrocatalyst for Low-temperature PEM Fuel Cell
P-105	Niharika Tanwar	Indian Institute of Technology, Guwahati	Sustainable Electrocatalytic Conversion of (M)ethanol to Sodium Carbonate: Leveraging Inexpensive 3d Metal Molecular Electrocatalysts
P-106	Deepak Aloysius	Indian Institute of Technology, Bhilai	Effect of PCBM Nanoparticles in Lead-based Layered (PEA) ₂ PbI ₄ Perovskite Thin Films
P-107	Dipti Ranjan Panigrahi	Shiv Nadar University, Greater Noida	Unraveling the Oxygen Reduction Reaction Activity Under Acidic Medium Using Designed N-doped Graphene Catalyst
P-108	Rajshree Rai	Banaras Hindu University, Varanasi	Ionic Liquid Assisted Single Sodium-Ion Conducting Styrene-Maleic Anhydride Copolymer for Energy Storage Application

P-109	Gokul Raj	Indian Institute of Science, Bangalore	Hydrolysis-Mediated Hydrogen Production using High Entropy Quintuple Alloy Grafted Carbon Black
P-110	Antony James	Indian Institute of Science, Bangalore	Enhancement of OER Activity of CuO _x on Incorporation of Lanthanides
P-111	Prathamesh Chougale	Jaysingpur College Jaysingpur, Kolhapur	Electrocatalytic Performance of Mn-doped Cobalt Ferrites for Water Splitting Applications
P-112	Ajinkya Kotkar	Indian Institute of Technology, Delhi	Green Recycling and Regeneration of Carbon-Coated LCO from Spent LIBs
P-113	Bhismadev Mahananda	National Institute of Technology, Rourkela	Anchoring Ni Doped Mn ₃ O ₄ on Bimetallic CoFe Layered Double Hydroxide for Efficient Electrocatalytic Oxygen Evolution Reaction
P-114	Vishal Rout	National Institute of Technology, Rourkela	Detailed Electrochemical, Synchrotron and DFT Investigations into the Enhanced Solar Promoted Photocatalytic Mitigation of Chloramphenicol and H ₂ Evolution by CuNi Alloy Bimetallic Nanoparticle Modified on h-BN Doped g-C ₃ N ₄
P-115	Smruti Vardhan Purohit	CSIR - Institute of Minerals and Materials Technology, Bhubaneswar	Selective Electrochemical Nitrogen Reduction to Ammonia by an Organic-Inorganic Hybrid Microporous Vanadium Phosphonate Material via the Distal Mechanism
P-116	Dineshkumar Yadav	Tata Institute of Fundamental Research, Mumbai	Gold Nanoparticles: Revolutionizing Bio-Electrolysis Efficiency
P-117	Priyanka Kumari	Vellore Institute of Technology, Vellore	Mechanical Milling Induced Synthesis of α -mZn/Co-ZIF-8 For Enhanced Electrochemical Water Splitting
P-118	Raghavakrishna Kanala	CSIR -Central Electrochemical Research Institute, Karaikudi	Metal oxide Functionalized Hollow Carbon Spheres as Electrocatalysts for CO ₂ Reduction
P-119	Asit Prakash	Indian Institute of Technology, Kanpur	Atmospheric Pressure Plasma Surface Modified Separator for Lithium Ion Battery
P-120	Naga Keerthana Apparla	Indian Institute of Technology, Hyderabad	High-Performance Symmetric Dual-Carbon Lithium-Ion Capacitor with Graphitized and Activated Carbon Xerogel Electrodes
P-121	Sruthi V.P.	Vellore Institute of Technology (VIT), Vellore	Prudently Designed Se@fMWCNT as Peroxidase Mimicking Nanozyme for Distinctive Electrochemical Detection of H ₂ O ₂ and Glutathione
P-122	Ruchi Agarwalla	CSIR-North East Institute of Science and Technology, Jorhat	Nitrogen-Doped Ti ₃ C ₂ MXene Quantum Dots/ MoSe ₂ Heterostructure: A New Avenue for Efficient Water Splitting
P-123	Riya Das	CSIR-North East Institute of Science and Technology, Jorhat	Evidence of Bimetallic Cooperativity in Water Oxidation Catalysis: The Key Role of Second Metal
P-124	Sony K. Cherian	Indian Institute of Technology, Hyderabad	Synergistic Effects of Nitrogen and Sulfur Co-doping in Xerogel Derived Hard Carbon for High-Performance Lithium-Sulfur Batteries
P-125	Shaswat Srivastava	Indian Institute of Science, Bangalore	Re-Nucleation and Re-Precipitation in Soluble Lead Redox Flow Battery
P-126	Soumalya Debnath	Indian Institute of Science Education and Research, Kolkata	Exploring the Electrocatalytic Superiority of Cobalt and Iron Based Precatalytic Oxalate Framework towards Alkaline Water Oxidation
P-127	Santanu Pal	CSIR -Central Mechanical Engineering Research Institute, Durgapur	Manipulation of Interfacial Electronic Structure of NiFe LDH/Ni ₃ S ₂ Heterostructure for Corrosion Resitive Sustainable Seawater Electrolysis
P-128	Ashwini Anshu	Indian Institute of Science, Bangalore	Bimetallic Alloy Nanoparticle Embedded N-Doped Carbon Nanotube for Electrocatalysis and Zn-Air Batteries
P-129	Ankit Kumar Verma	Indian Institute of Science, Bangalore	Overcoming Activity-Stability Tradeoff in Water Splitting Catalysis: Lower Overpotential and Higher Stability of Ni-doped MoO ₃ for Alkaline Oxygen Evolution
P-130	Varun Natu	National Chemical Laboratory, Pune	Engineering MXenes to Boost their Performance in Batteries
P-131	Rupali Mane	Institute of Chemical Technology, Mumbai	N-doped Norbornane SP ² Carbon Framework: An efficient electrocatalyst for Oxygen Reduction and Hydrogen Evolution Reaction
P-132	Nasir Ali	Indian Institute of Technology, Roorkee	Fabrication and Characterization of Functionalized Metal-Organic Framework Embedded Proton Exchange Membranes for Green Hydrogen Production in PEM Water Electrolyzer
P-133	Sarvesh Kumar	Indian Institute of Science, Bangalore	Nickel-Embedded Carbon Nanostructures as Noble Metal-Free Catalysts for the Hydrogen Evolution Reaction
P-134	Joel John	Indian Institute of Science Education and Research, Mohali	Electronic Redistribution through the Interface of MnCo ₂ O ₄ -Ni ₃ N Nano-Urchins Prompts Rapid in Situ Phase Transformation for Enhanced Oxygen Evolution Reaction
P-135	Palash Jyoti Medhi	Institute of Advanced Study in Science and Technology, Guwahati	Ruthenium Nanoparticles onto MXene through “Defect Engineering” to Enhance the Activity of the Hydrogen Evolution Reaction in Alkaline Medium
P-136	Diya Raveendran	Indian Institute of Science Education and Research, Kolkata	Lattice Engineering Triggered Phase Formation of Bimetallic Thiospinels with Excellent H ₂ OR Activity for Energy-Efficient Hydrogen Production

P-137	Karthick Raja K	Indian Institute of Information Technology Design and Manufacturing, Chennai.	Investigating Electrochemical Performance of MIL-100(Fe)@ CoSn(OH) ₆ for Asymmetric Hybrid Supercapacitor
P-138	Riya Anilkumar Javiya	Indian Institute of Technology, Gandhinagar	Effect of pH on Hydrogen Production from Formic Acid and Study of Role of Pd Based Catalysts
P-139	Gayatri Neog	Institute of Advanced Study in Science and Technology, Guwahati	High Entropy Oxide towards Electrochemical Oxygen Evolution Reaction
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P-141	Sambhaji Pawar	Sanjay Ghodawat University, Kolhapur	Highly efficient Mo Doped CuNiFe Based Metal Organic Framework (MOF) Catalyst for overall Water Splitting Application
P-142	Geetanksha Gupta	Indian Institute of Technology, Bombay	Kinetic Study of Hydrogen Oxidation/Evolution Reactions on Nickel in Alkaline Medium
P-143	Avoy Mondal	Indian Institute of Technology, Delhi	Durable, Efficient, and Cost-Effective Anion Exchange Membrane in An Affordable Alkali Water Electrolyzer for Green Hydrogen Production
P-144	Ashish Kumar Yadav	Rajiv Gandhi Institute of Petroleum Technology, Amethi	Highly Dispersed Ultrafine FeNi-Phosphide Nanoparticles Embedded in Amorphous FeNiO _x For Oxygen Evolution Reaction
P-145	Padmavathy B	Indian Institute of Technology, Palakkad	Ni/NiO/N doped Graphene Coated Nickel Foam for Advancing Urea Degradation and Hydrogen Production in Urea-Enriched Wastewater
P-146	Rubul Das	Indian Institute of Technology, Bombay	Temperature-dependent Investigation of ORR Kinetics on Non-Precious Metal-free Catalysts in Alkaline Media - Doping Effect on Electrocatalysis
P-147	Santosh Semwal	Rajiv Gandhi Institute of Petroleum Technology, Amethi	Surface Mediated Growth of Polyacryloyl Hydrazide Promoted Co ₃ O ₄ @NiCu Alloy Nanocuboids for Alkaline Methanol Oxidation Coupled H ₂ Production
P-148	Amit Kumar	Institute of Engineering and Technology, Lucknow	Carbon-Negative eFuel: Advancing Direct Air Capture with Saltwater Electrolysis
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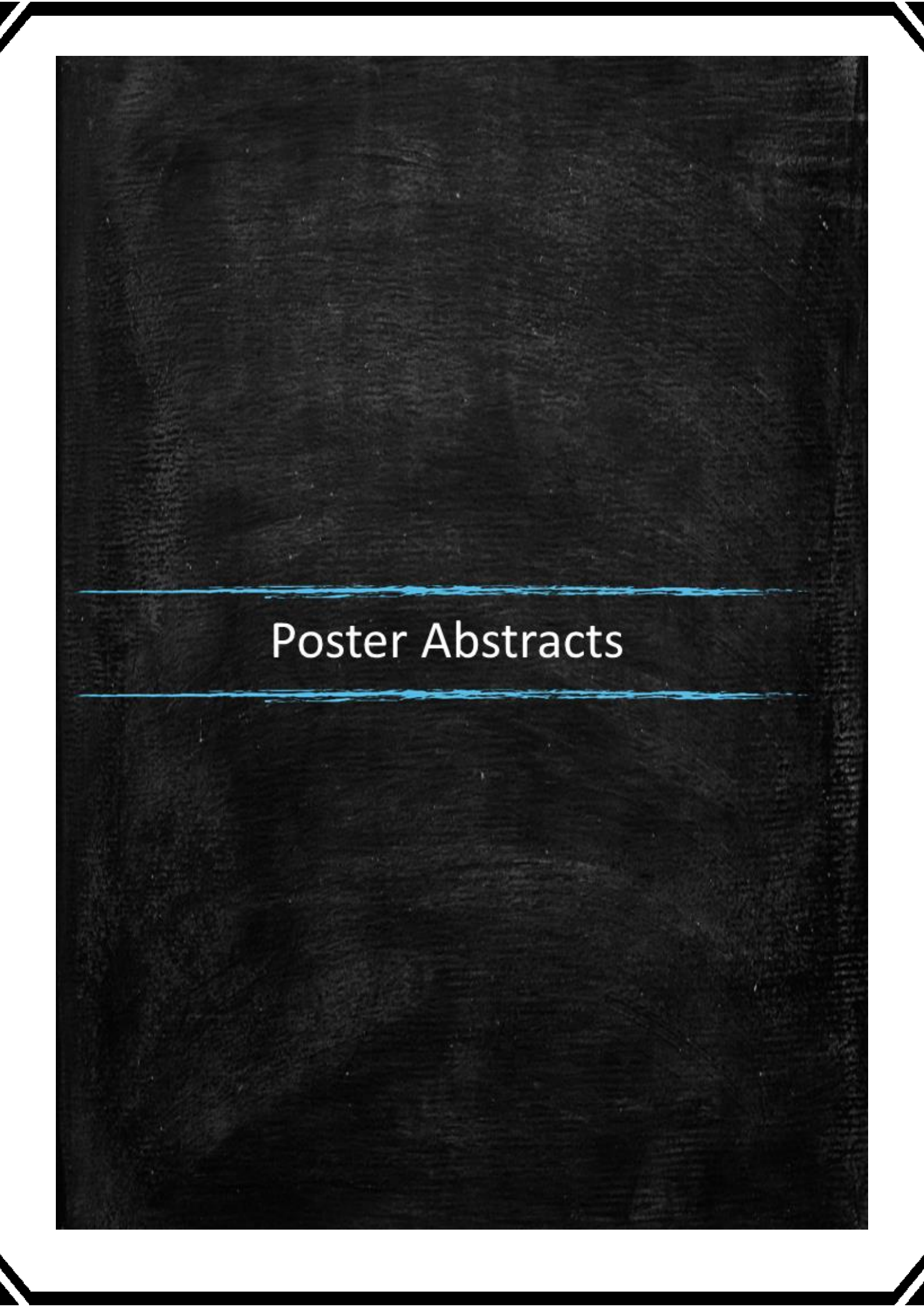
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P-305	Rishi Verma	Tata Institute of Fundamental Research, Mumbai	Harnessing Plasmon-Enhanced Hot Electrons for Solar-Driven Catalysis in Black Gold-Nickel Systems
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P-307	Twinkle Jain	Indian Institute of Technology, Delhi	Shell Passivation in Perovskite Nanocrystals: Improving Stability and Optical Properties with Lead-Free Cs ₃ Bi ₂ Br ₉ Coating
P-308	Praduman Gupta	Indian Association for the Cultivation of Science, Kolkata	Monodispersed PdO Nanoparticles on the Surface of Polyaniline Nanotube and its Efficient Electrochemical Hydrogen Evolution



Poster Abstracts

Selective Metal-Free CO₂ Photoreduction in Water Using Porous Nanostructures with Internal Molecular Free Volume

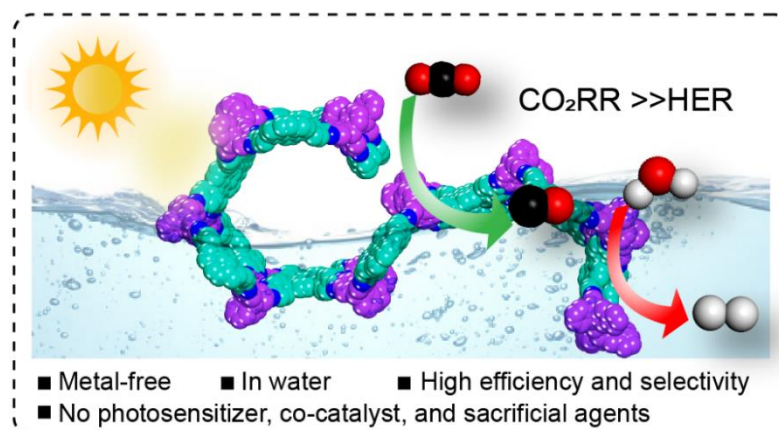
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Abstract

The conversion of CO₂ into a single carbonaceous product *via* photocatalysis offers a sustainable way to reduce CO₂ emissions and lessen reliance on fossil fuels.¹ However, developing an efficient, metal-free catalyst for CO₂ reduction (CO₂RR) that doesn't require sacrificial agents, cocatalysts, or photosensitizers is challenging.² The poor solubility of CO₂ in water and the favored hydrogen evolution reaction (HER) complicate the design of selective photocatalysts.³ In this study, we use molecular engineering⁴ to design a photoactive polymer with high CO₂ permeability and low water diffusivity, enhancing CO₂ mass transfer while suppressing HER.⁵ We incorporated a contorted triptycene scaffold with internal molecular free volume (IMFV) to create molecular channels, improving gas permeability. A pyrene moiety was also introduced to enhance visible light harvesting and charge separation. This polymer achieved a CO generation rate of 77.8 $\mu\text{mol g}^{-1} \text{h}^{-1}$, with ~98% selectivity and good stability for five cycles. Replacing the triptycene unit with a planar scaffold reversed the selectivity, favoring HER over CO₂RR.



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Solid Oxide-Based Electrodes for CO₂ Reduction

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Abstract:

Converting CO₂ into fuels can substantially reduce our dependence on fossil fuels. One efficient method involves the high-temperature electrochemical reduction of CO₂ to CO using a solid oxide electrolysis cell. The resulting CO can either be used directly or converted into higher hydrocarbons through the Fischer-Tropsch process. However, current cathode catalysts such as Ni, CeO_x, and perovskites are hindered by slow reaction kinetics and deactivation issues, including coking.

To address these challenges, we have developed a novel 2-chamber high-temperature operando setup that integrates Raman spectroscopy, online mass spectroscopy, optical microscopy, and electrochemical measurements. This setup enables us to observe catalysts in real time, monitoring their structural changes during the reaction and correlating these changes with activation and deactivation phenomena. Using this setup, we have investigated two types of electrodes, Ni{M}_x-YSZ, and Ce{M}O_x-YSZ, under both pure CO₂ and CO₂ (+H₂) streams.¹⁻⁴

Our research has provided new insights into catalyst activity and stability, and we have successfully mitigated several challenges through catalyst modification and process optimization.

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Flue Gas Reforming of Methane using Ni-Al₂O₃ and Ni-Co-Al₂O₃ Catalysts

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Abstract

Flue gas reforming of methane (FGRM) involves the co-feeding of methane to industrial flue gas to convert CH₄ and CO₂ into hydrogen and syngas (a mixture of CO and H₂). In this study, a series of Ni-Al₂O₃ and Ni-Co-Al₂O₃ catalysts were synthesized, characterized, and tested for FGRM at 600°C under atmospheric pressure. These catalysts were calcined at 850°C to take advantage of strong metal/alloy-support interactions (SMSI). The effect of metal loading, reduction temperature, and cobalt promotion on catalyst activity and stability were investigated to determine the most suitable catalyst formulation for FGRM. The results revealed that high-temperature calcination resulted in excellent catalytic stability. Reducing the fresh catalysts using pure H₂ at their respective maximum reduction temperatures (T_{max}) from H₂-TPR profiles led to a higher number of surface sites than any other temperatures. The catalytic performance of Ni-Al₂O₃ varied with change in the metal loading and 15wt.% Ni-Al₂O₃ showed the optimum catalytic performance. An enhancement in the catalytic activity of Ni-Al₂O₃ was achieved by strategically substituting Ni with Co using the bimetallic Ni-Co-Al₂O₃ catalysts. An increased and stable CH₄ (89%) and CO₂ (30%) conversions and H₂ (79%) and CO (46%) yields with desired H₂/CO molar ratios (≥3) in the syngas were achieved using 10wt.% Ni₃Co-Al₂O₃ catalyst. A microkinetic model was also developed and validated for the FGRM process. The proposed model was able to correctly predict the reactant conversions and product yields across various contact times and temperatures. Thus, the catalyst synthesis and activation parameters, along with the promoters, play a crucial role in developing a highly active, stable, and durable catalyst for a carbon-free and energy-efficient FGRM process at relatively low temperatures.

Acknowledgments

I would like to express my deepest gratitude and sincere thanks to my thesis supervisor, Prof. Goutam Deo from IIT Kanpur, for their invaluable guidance, critical insights, and unwavering support throughout my PhD journey. I am also profoundly thankful to Dr. Vaibhav Kumar Arghode from the Sustainable Energy Engineering Department IITK for his valuable guidance and generous support. Additionally, I extend my heartfelt appreciation to my lab mates, especially **Russel** and **Saumya**, for their constant support, encouragement, and assistance whenever I needed it.

Exploring Bis-NHC Amino Pincer Ligand-Based Bifunctional Ru and Mn Complexes toward Catalytic Hydrogenation of CO₂

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Abstract

Research on capture and catalytic conversion of CO₂ to valuable chemicals and alternative fuel candidates has multifaceted relevance from the perspective of sustainable development goals (SDGs). Methanol, advocated as an alternative fuel, can be produced via amine-assisted integrated capture of CO₂ and the subsequent hydrogenation via formamide intermediate. Structurally well-defined, transition metal-based efficient and sustainable hydrogenation catalysts are of special interest in this regard. However, most of the reported efficient molecular catalysts are based on expensive and air-sensitive phosphine-based ligand systems. Hence, alternative ligands are of paramount interest and can play an important role in this research problem. The key emphasis of this work is to rationally design and develop stereoelectronically-balanced N-heterocyclic carbene (NHC)-based metal complexes suitable for efficient catalytic hydrogenation of CO₂. With the above goal in mind, a "bis-NHC amino" pincer ligand (**L1**) based on imidazo[1,5-*a*]pyridine-3-ylidene (**ImPy**) has been designed through a rational mechanism-guided approach to develop its Ru and Mn complexes for the target CO₂ hydrogenation catalysis. The proton-responsive bifunctional nature and an appropriate electronic attribute of the **L1** ligand, as discovered in these projects, triggered to develop a highly competent Ru(II)-based alternative catalyst for the CO₂-to-MeOH conversion protocol using a regenerable amine, which was then translated into a porous hypercrosslinked polymer (HCP)-based self-supported single-site heterogeneous catalyst, termed as **HCP-Ru-1**. Initially, control mechanistic investigation was performed in order to get insights into the crucial H₂ activation step at the Ru centre of the catalyst assisted by the amine used in the reaction. Finally, for the catalytic CO₂-to-MeOH production reaction, a polyamine pentaethylenehexamine (PEHA) was used due to its high efficiency in CO₂ capture as well as ability to act as a suitable organic base for deprotonative H₂ activation, and significantly the **Ru-1** and **HCP-Ru-1** systems displayed a single-run TON of 400 and 1150 respectively. As the most significant advancement in this process, the heterogeneous **HCP-Ru-1** catalyst turned out to be highly reusable and in a 10-cycle reuse demonstration experiment, it achieved a cumulative TON of 10370 with merely 1.13% loss in activity per cycle. Mn(I) bis-NHC amino pincer complex was found to be equally active toward sequential hydrogenation of CO₂ to methanol via formamide intermediate, providing a very good catalytic turnover.

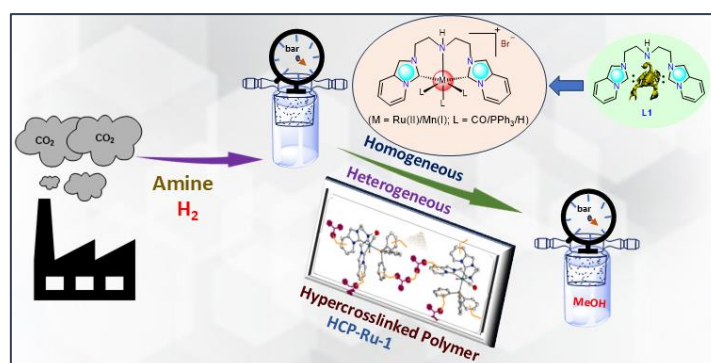


Figure 1. Schematic representation of CO₂ to methanol transformation using Ru and Mn catalysts

A DFT study of biomimetic CO₂ hydration reaction on high-index Ni (211) surface

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Abstract

Development of carbon-neutral energy systems for a sustainable future has become imperative considering increased CO₂ concentration in the atmosphere from the use of conventional fuels. CO₂ hydration reaction (CHR¹⁻³) has been identified as potentially an important reaction for capturing CO₂ and its conversion to mineral carbonates. Pre-coverage of a clean Ni (211) surface with OH plays an important role in activating CO₂ molecules during a host of surface catalytic reactions involving CO₂ and H₂O and detailed understanding of the reaction will assist in developing improved catalysts. Density functional theory calculations were employed to investigate CO₂ capture via CHR with modified Ni (211) surface acting as biomimetic catalysts exhibiting carbonic anhydrase-like mechanism⁴. Appreciating this observation, the present work was designed to focus on providing detailed mechanistic insights into CHR reaction by Ni (211) surface, pre-covered by oxygenated surface species formed because of partial dissociation of H₂O. The binding energies of hydro-oxygenated species namely, H₂O, CO₂, and their derivatives, were determined. Potential energy surfaces were developed for the formation of bicarbonate for H-rich and H-depleted conditions. Our computational analysis conclusively demonstrates the feasibility of Ni (211) to act as heterogeneous biomimetic CHR catalysts which can potentially be implemented in industrial CO₂ capture setups.

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Mechanistic Investigation for CO₂ Hydrogenation to Methanol and Methanol Conversion to Hydrocarbons

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Abstract

Potential strategies like carbon capture, storage, and utilization are being explored to mitigate anthropogenic CO₂ emissions. This work focuses on the thermocatalytic conversion of CO₂ to produce value-added chemicals like methanol and hydrocarbons. Due to their high activity and stability, Cu/ZnO/ZrO₂/Al₂O₃ catalysts are widely explored for CO₂ conversion to methanol. Reactor experiments showed high variability in performance among the Cu-based catalysts due to differences in the catalyst structure. However, a mechanistic understanding of the performance of such multicomponent catalysts is lacking due to ambiguity on the catalyst structure and their actual active sites. The reactor level performance of these catalysts can be predicted only when the kinetic consequences arising from the surface of the catalyst nanostructure are investigated using a detailed DFT-based reactor scale microkinetic model.

The initial part of this thesis focuses on unraveling the role of various active sites, such as ZnO_x/Cu and ZrO₂/Cu interfaces, on Cu/ZnO/ZrO₂/Al₂O₃ catalyst by coupling experiments and DFT simulations. The analysis found the ZnO_x/Cu interface to be the prominent reaction center for methanol synthesis. This thesis also investigated the facet-dependent activity of the Cu/ZnO/Al₂O₃ catalyst arising from surface exposures of different Cu crystal facets in the metallic Cu component of the catalyst. ZnO_x/Cu(111) and ZnO_x/Cu(100) surfaces are catalytically relevant for CO₂ hydrogenation, with the ZnO_x/Cu(100) being more active.

CO₂ hydrogenation on tandem catalysts comprising a mixture of metal oxide and zeolite MeO_x/ZSM-5 (MeO_x – ZnO, ZrO₂, In₂O₃, and ZnZrO_x) have been explored to understand the influence of the cationic exchange with the Brønsted acid site (BAS) of HZSM-5 zeolite catalyst on the hydrocarbon distribution. The propensity for cationic exchange with the BAS of ZSM-5 was demonstrated as a function of the metal vacancy formation energy of MeO_x catalysts, which was high for ZnO and In₂O₃. Cation exchange and formation of In/ZSM-5 entities in the zeolite catalyst aids in methane formation via methanol hydrogenolysis, whereas Zn/ZSM-5 enhances paraffin selectivity while inhibiting C₅ species formation.

Overall, this thesis offers a comprehensive exploration of CO₂ utilization to methanol and methanol conversion to hydrocarbons, employing first principles DFT simulations to understand the mechanisms and reaction behavior. This work would help develop strategies for catalyst design for converting CO₂ to potential chemicals towards a sustainable low-carbon future.

Keywords: Density Functional Theory, Methanol production, Multicomponent catalyst, CO₂ hydrogenation, Methanol to Hydrocarbons, Metal Modified ZSM-5

DFT and ML Methods for Screening of Homogeneous/Heterogeneous Catalysts for C₁/C₂ Products from CO₂

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Abstract

The catalytic CO₂ reduction reaction (CO₂RR) is pivotal for progressing toward carbon neutrality while simultaneously producing valuable chemicals and fuels such as HCOOH, CH₃OH, C₂H₄, C₂H₅OH, and others. Both homogeneous and heterogeneous catalysts have shown great potential in facilitating these transformations. In this thesis, a comprehensive approach combining density functional theory (DFT) and machine learning (ML) is adopted to investigate the most favorable pathways for CO₂ hydrogenation reactions. The study also explores the effect of various ligands on homogeneous catalysts, specifically targeting C₁ product formation, with a focus on optimizing their performance. Furthermore, for the heterogeneous CO₂RR, the thesis proposes the use of specific additives and introduces single-atom alloy (SAA) and dual-atom alloy (DAA) catalysts aimed at enhancing C₂ product formation (Figure 1). The accomplishments include significant improvement in catalytic activity, particularly in C₁ product (CH₃OH) formation with the use of earth abundant Mn based homogeneous catalysts, driven by ligands with strong electron-donating (+I) effects. A novel ligand-encoded feature matrix have been introduces to screen suitable catalysts with significant accuracy. The early group transition metals proposed to be suitable dopants for SAA and DAA catalysts to obtain selective C₂ products. These findings present promising pathways for efficient CO₂ utilization, addressing both environmental and industrial demands.

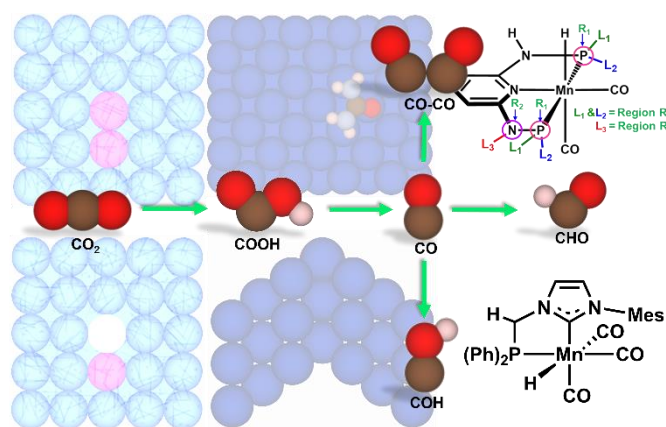


Figure 1. The figure representing all the considered catalysts for CO₂ reduction reaction in the thesis.

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Optimizing Heterogeneous Photocatalyst Design for CO₂ Reduction to Fuels

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Abstract

The challenge of converting CO₂ into valuable products through photocatalysis is pivotal to realizing a sustainable, circular carbon economy. This research addresses critical barriers that impede the industrial scalability and practical application of this technology, including the limited effectiveness of photocatalysts, marked by low activity and selectivity, essential for high-yield production of chemicals like methane, syngas, and methanol. Additionally, the reliance on costly, rare materials for catalyst synthesis escalates costs and hinders widespread adoption. A significant gap in understanding the molecular mechanisms of CO₂ reduction complicates the rational design and optimization of effective photocatalysts, particularly under real-world sunlight conditions characterized by low-intensity light. Addressing these material and technical challenges is crucial for advancing CO₂ photoreduction from a theoretical concept to a viable industrial application, essential for reducing environmental impact and enhancing energy security. Significant advancements were achieved that enhanced the efficacy and scalability of photocatalytic materials for CO₂ reduction. A pivotal part of the work involved exploring the photocatalytic potential of carbon nitride (CN) materials, prized for their cost-effectiveness and ease of synthesis. Through strategic defect engineering, a significant boost in photoactivity was achieved, highlighting the essential role of defects in enhancing photocatalyst performance. However, the structural complexity of CN and the challenges it presents for rational modifications underscored the need for advanced characterization methods. To address this, a computational approach based on quantum calculations and vibrational mode analysis was introduced, enabling the identification of a metastable, undulated form of carbon nitride. This form exhibited high photocatalytic activity due to stabilized CO₂ interactions and extended charge carrier lifetimes. Further research developed a heterojunction consisting of MoS₂ and Cu₂O, integrated via a Z-scheme charge transfer mechanism. This innovative configuration significantly improved methanol production compared to using MoS₂ or Cu₂O individually, highlighting the importance of composite catalysts and charge transfer modulation in enhancing photocatalytic efficiency. Additionally, studies extended to the role of metal dopants in TiO₂, a widely used catalyst in photocatalysis. Employing in-situ Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS), the molecular-level reaction mechanisms were dissected, revealing how specific metal dopants selectively improve reaction pathways, thus enhancing both the selectivity and efficiency of CO₂ reduction. Photocatalytic CO₂ reduction technology is currently poised at a critical juncture, requiring significant technological advancements to transition effectively to industrial-scale applications. This research has focused on pioneering these advancements by deepening the understanding of the complex interactions among materials and light, as well as between reactants, products, and charge carriers. By leveraging low-cost materials and implementing innovative catalyst designs, essential challenges in cost, efficiency, and practical deployment have been addressed. The detailed mechanistic insights gained from spectroscopic analyses and kinetic modeling have substantially propelled the field forward, facilitating the rational design of more effective photocatalysts. Moreover, investigations into perovskite materials have enhanced performance under variable lighting conditions, significantly broadening their applicability across various geographic settings. This work not only improves the adaptability of the technology but also extends its accessibility on a global scale, underscoring its potential to transform the energy landscape and effectively mitigate environmental impacts.

Hydrate Formation in the Presence of Promoters for CO₂ Capture and Storage Application

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Abstract

The rapid increase in world energy demand is leading to a significant rise in CO₂ emissions to the atmosphere. CO₂ emissions have drastically increased in India over the years, making it the world's third largest CO₂ emitter after China and the USA. Therefore, CO₂ capture and storage technologies have become very important for mitigating CO₂ from the environment. The gas hydrate technology can be used as an alternative approach for CO₂ capture and storage applications. There are several advantages of gas capture and storage using hydrate-based techniques, including an environment friendly approach, no use of hazardous chemicals, easy gas recovery, and a moderate temperature and pressure requirement for hydrate formation. The present thesis focuses on enhancing the kinetics of CO₂ hydrate formation in the presence of promoters for CO₂ capture and storage applications. The experiments were conducted at 275.15 K temperature and 3.0 MPa pressure in both lab-scale (150 ml) and pilot-scale (25 L) stirrer reactors. Different types of kinetic (Cu-Al LDH nanofluid and methionine) and thermodynamic promoters (THF and CP) were utilized to improve CO₂ hydrate formation kinetics.

A cost-effective hybrid nanofluid (Cu-Al LDH) was prepared using a one-step co-precipitation technique and subsequently used as a kinetic promoter for CO₂ hydrate formation. The shape/size, structural features, thermal property, and suspension stability of LDH nanoparticles/nanofluid were characterized using TEM, XRD, thermal conductivity, and zeta potential measurement. The hydrate formation experiments were conducted in a pilot-scale reactor for different LDH nanofluid concentrations (0.25-1.0 wt%) and molar ratios (Cu²⁺:Al³⁺: Na⁺ = 4:1:4 and 4:1:4.7). The addition of the LDH nanofluid enhanced the gas absorption and hydrate formation process. The CO₂ hydrate formation kinetics was enhanced with an increase in LDH nanofluid concentration up to an optimum concentration, beyond which the hydrate formation kinetics was reduced. The morphology of hydrate formation changed with an increase in the molar ratio of the LDH nanofluid. The results demonstrated a strong dependency of elemental molar composition and LDH nanofluid concentration on the overall gas absorption and hydrate formation process.

The effect of kinetic (L-Met) and thermodynamic (THF and CP) promoters on the CO₂ hydrate formation kinetics was investigated in a lab-scale reactor. The experiments were conducted at fixed thermodynamic promoter concentration (1.0 mol%) and systematic variation in the kinetic promoter concentration (0.05-0.5 wt%) to evaluate the synergistic effect of the promoters on the hydrate formation kinetics. The experimental results revealed that thermodynamic promoters (THF and CP) drastically reduced the induction time compared to DI water system. However, the combined use of the thermodynamic and kinetic (THF+L-Met and CP+L-Met) promoters showed no synergistic effect on the induction time. The gas consumption was significantly enhanced in the presence of combined thermodynamic and kinetic promoters, demonstrating the synergistic effect of both promoters on improving hydrate formation kinetics. The combined use of promoters induced hydrate growth on the reactor wall through capillary action. The electrical energy consumption analysis demonstrated that the presence of thermodynamic promoters (THF and CP) reduced the energy consumption for hydrate formation.

Synthesis and Characterization of Adsorbents for Direct Air CO₂ Capture

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Abstract

The present research focuses on the development of advanced adsorbents for direct air CO₂ capture (DAC), a critical technology for addressing the rising atmospheric CO₂ levels. The key objectives of this work include utilizing the large surface area and unsaturated open metal sites in Metal Organic Frameworks (MOFs), particularly MIL-101(Cr), combined with rice husk ash (RHA), an agricultural waste material as a silica source. This approach creates ultra-microporosity, significantly enhancing CO₂ adsorption characteristics such as working capacity, purity, and the ability to capture CO₂ under humid conditions. The research also designs structured adsorbents for practical, large-scale industrial DAC applications.

In addition, this study explores the challenges associated with amine modification of silica for capturing CO₂ from simulated (≥ 400 ppm CO₂ in helium) and indoor air environments. A sustainable solution is provided to address issues such as slow CO₂ adsorption kinetics, high moisture sensitivity, high regeneration temperatures, and low thermo-cyclic stability. Notably, nano silica dendrimers were developed, offering improved adsorption performance and durability in cyclic operations.

A key achievement of this work is the utilization of regenerated CO₂ for the formation of value-added products such as formate and calcium carbonate (CaCO₃) pellets. These products not only offer sustainable pathways for CO₂ utilization but also enhance the overall economic viability of the DAC process.

The overarching goal is to develop affordable, bulk-scale adsorbents in structured forms, capable of substantial CO₂ uptake under both dry and humid conditions, without capacity loss during prolonged cyclic adsorption-desorption processes. This research presents a practical and scalable solution for CO₂ capture, contributing to the circular economy and sustainable industrial practices by not only mitigating atmospheric carbon levels but also converting captured CO₂ into valuable products, paving the way for a cleaner and more economically viable future.

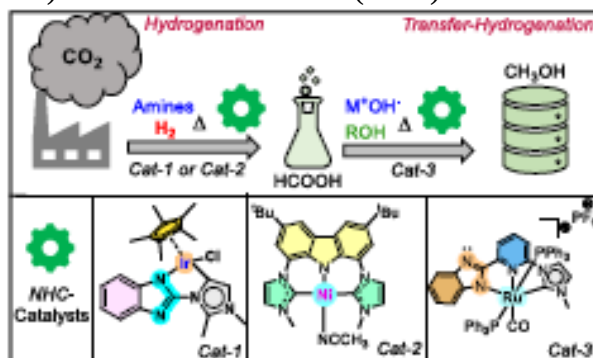
Integrated CO₂ Capture and Conversion: Probing NHC-Based Organometallic Catalysts

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Abstract

Carbon capture and utilization (CCU) with its aim to convert the captured carbon dioxide into more valuable chemicals has been heralded as an opportunity to develop a sustainable economy. C1 products such as formic acid and methanol which can be obtained from CO₂ through CCU have a varying multitude of usages. Formic acid is used as a preservative and antibacterial agent in livestock feed. It is also used in the production of leather, dyeing, and finishing textiles. More recently, it has also gained interest as a hydrogen energy carrier owing to its liquid nature and high volumetric capacity (53 g H₂ L⁻¹). Methanol has long been advocated as a convenient liquid fuel/fuel substitute/fuel additive and is used as a raw material for synthetic hydrocarbons. In the past decade a handful of homogenous catalysts have been reported for CO₂ capture and hydrogenation to C1 products. These catalysts are mostly based on air-sensitive and expensive phosphine-based ligand systems. N-heterocyclic carbenes (NHCs) serve as a versatile class of strong σ -donor ligands in transition metal-based several hydride-transfer catalyses and are a great substitute for phosphine-based ligands. Coupled with the NHC ligands, utilization of non-noble metal-based catalyst systems and renewable H₂-surrogates such as alcohols for CO₂ reduction processes, leaves a lot of opportunity for further innovative investigation. With the abovementioned opportunities in consideration, this thesis covers the study of amine-assisted integrated CO₂ capture and hydrogenation (CCH) to formate using a phosphine-free “benzimidazolato-*abnormal* NHC”-based molecular Ir catalyst under an all-aqueous conditions. This system serves as not only the first phosphine-free module for such transformation but also as the only all-aqueous system. On the other hand, base-metal catalysts (Co, Fe, Ni) are less explored for the hydrogenation of CO₂ to formate. In particular, Ni-based systems exhibit some unique challenges in this regard associated with the hydride-formation and hydride-delivery of the Ni–H species. With the help of a rationally-designed “carbazolato-*bis*-NHC”-based tridentate chelating ligand, a Ni-NHC catalyst was developed and utilized efficiently in the abovementioned CCH protocol. Furthermore, in the domain of highly important CO₂-to-MeOH (CTM) process, an indirect strategy was explored by employing HCOOH as the intermediate substrate, after a successful demonstration of an unprecedented integrated CO₂ capture and transfer hydrogenation (CCTH) method. For this purpose, easily available alkali metal hydroxides and renewable (bio)alcohols were employed to convert HCOOH to MeOH, by using a “benzimidazolato-pyridine-NHC”-based chelating ligand-bound Ru catalyst. Transfer hydrogenation of formic acid to methanol using a renewable alcohol has not been attempted yet and this work serves as its first exploration. These studies offer some key insights into the important and challenging CO₂-to-formate (CTF) and CO₂-to-methanol (CTM) conversion protocols.



I. An all-aqueous and phosphine-free integrated amine-assisted CO₂ capture and catalytic conversion to formic acid

Elucidation of the Mechanisms Behind Selective Oxidation of Methane to C1 and C2 Oxygenates Over FeAu/ γ -Al₂O₃ Catalysts

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Abstract

Partial oxidation of methane to methanol and other oxygenates without the formation of CO₂ is highly desirable^{1,2,3}. In this work, we demonstrate a green synthesis protocol for preparing gold nanoparticles supported on alumina (Au/ γ -Al₂O₃) and iron oxide promoted on Au/ γ -Al₂O₃ catalysts. Aqueous phase methane oxidation reaction was performed using these catalysts with O₂. Experimental results confirm that the Au/ γ -Al₂O₃ and Fe/ γ -Al₂O₃ catalysts displayed high selectivity for C₁ oxygenates such as HCOOH, HCHO, and CH₃OH at a mild temperature of 75 °C. In contrast to the single-metallic catalysts, the iron oxide-promoted gold alumina (bimetallic) catalysts “FeAu/ γ -Al₂O₃” selectively form ethanol (95% selectivity, ~240 μ mol per gram of catalyst). Characterization results confirm that the iron-oxide promotion on the gold leads to an anionic character while making it smaller in size, which is responsible for the selective formation of ethanol. DFT results confirm the intermediates for ethanol formation are more favorable than methanol on FeAu/ γ -Al₂O₃. We conclude from the DRIFTS and DFT mechanistic investigations that FeO_x-Au interfaces enable methane activation across the interface, and the coupling step happens on the gold nanoparticle. The reaction mechanism follows via the CH₂OH intermediate is the most likely route for ethanol formation on the bimetallic catalyst.

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Carbon dioxide Transformation to Sustainable Energy and Fuels using Low coordinated Molecular Catalyst

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Abstract

Methanol stands as one of the foremost commodity chemicals, with an annual production exceeding 70 million tons, positioning it as a preeminent CO₂-derived C1 building block.¹ In light of the escalating demand for methanol as an alternative fuel, the pursuit of a cost-effective, sustainable, and scalable production methodology from renewable sources emerges as a paramount objective. Addressing current challenges, we have successfully synthesized a robust cobalt-based metal catalyst, [Li(DME)₃][Co(L1)₃], characterized by low coordination and exceptional reactivity.² This catalyst effectively converts thermodynamically stable CO₂ into trimethoxy borane using NaBH₄ as hydride source, which hydrolyzes to yield methanol under mild conditions. Our catalyst achieved high Turn Over Numbers (11,171) and Turn Over Frequencies (508 h⁻¹), along with notable longevity. The superior reactivity is attributed to the catalyst's coordinatively unsaturated site around Co(II), which contrasts with more stable geometries like octahedral and tetrahedral structures. We systematically intercepted intermediates in the catalytic cycle using NMR and ESI-MS, demonstrating that this catalytic method could potentially reduce CO₂ from vehicle exhaust (containing CO₂, CO, NO_x, and other hydrocarbons). With a TOF of 3000 h⁻¹, our work underscores the importance of coordination around 3d-metal centers in achieving high CO₂ to methanol conversion rates, comparable to heterogeneous catalysts, under mild conditions.

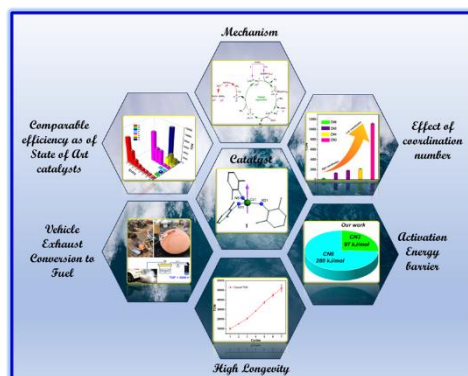


Figure: Graphical representation revealing highlights of our CO₂ to methanol conversion

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Thermocatalytic CO₂ Utilization by Oxidative Dehydrogenation of Propane using Mixed Metal Oxides: An Alternative Approach to CrO_x Based Catalysts

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Abstract

Utilization of CO₂ in a light alkane dehydrogenation reaction is one of the promising oxidative routes currently explored for enhancing olefin yield with a high CO₂ conversion rate. The conversion of CO₂ to CO through reverse water gas shift (RWGS) reaction makes this process economically efficient for the use of CO as a platform compound. Despite years of research, metal or metal oxide-based oxidative dehydrogenation is not yet commercialized. The primary challenge lies in effective adsorption and activation of propane and CO₂ on a single metal or metal oxide surface. Owing to this, we have attempted to synthesize bulk and supported mixed metal oxide (MMO), a series of novel catalysts which can ensure continuum of redox cycles of active metal during CO₂-oxidative dehydrogenation of propane. Our preliminary results showed that FeCr, one of the bulk MMOs, is associated with higher initial propane conversion, propylene formation and selectivity due to Fe-Cr synergism. Addition of Fe into Cr significantly reduced the apparent activation energy compared to Vanadium addition. To ensure thermostability of FeCr, supported catalysts were prepared using TiO₂, Al₂O₃, SiO₂, and CeO₂ supports. Overall, Al₂O₃-supported FeCr was found to be significantly active, selective and stable than the rest.

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CO₂ Hydrogenation to Formate by Molecular Ir Complex-Based Polymeric Catalyst

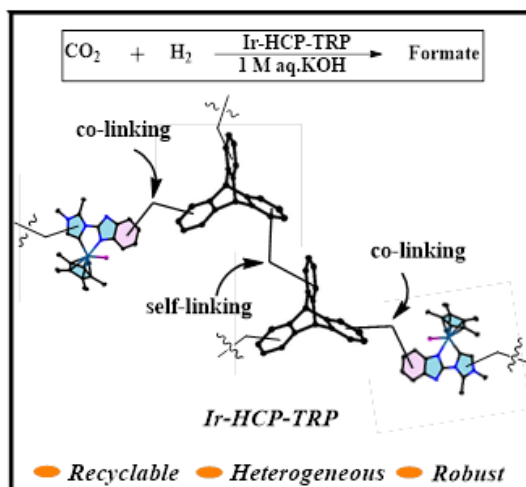
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Abstract

Integrated strategies for carbon capture and sequestration (CCS) and carbon capture and utilization (CCU) are used to remove CO₂ from both point sources (like industrial facilities) and diffused sources (such as the atmosphere)¹. Under CCU, hydrogenation of CO₂ using inorganic bases like NaOH and KOH results in inorganic formates which can be used, without purification, in direct formate fuel cell (DFFC)². Therefore, hydrogenation of CO₂ using NaOH/KOH as the base in aqueous medium to produce sodium/potassium formate salts is of paramount interest. Recently, our group demonstrated hypercrosslinked polymer (HCP)-based polymeric catalysts for CO₂ hydrogenation to methanol³ and formate⁴. For formate production, our previously reported molecular Ir-aNHC catalyst was heterogenized using triphenylmethane as copolymerizing agent. The polymeric catalyst **Ir-HCP-TPM** showed excellent reusability furnishing a cumulative TON of 285400 in 10 cycles. Here, to improve CO₂ adsorption capacity we heterogenized Ir-aNHC catalyst using a rigid molecule with a 3D skeleton triptycene. The heterogenized catalyst **Ir-HCP-TRP** with low loading (0.005 μmol of Ir) gives 2752 μmol of formate with a TON of 550400 in 12 hours. After 10 catalytic cycles, we got cumulative TON of 1414328 with 0.05 μmol of Ir loading with just 1.3 % loss in catalytic activity per cycle, which confirms the robustness of catalyst.



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Kinetic and Mechanistic Study of Structured Catalyst for Dry Reforming of Methane Reaction

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Abstract

Methane and Carbon dioxide are prominent greenhouse gases and can be converted to useful Synthesis Gas (Hydrogen and Carbon monoxide) using Dry Reforming of Methane (DRM) reaction. DRM has been investigated for many years and yet not commercialized. This process is catalyzed by Nickel based catalysts on different supports as Ni is widely known for reforming. In this study, we utilized in-situ infrared (IR) spectroscopy to explore the surface reaction mechanisms occurring on a structured catalyst. Kinetic experiments were conducted over a temperature range of 600°C to 800°C for the same catalyst. The experimental data were modeled using generalized rate equations, which were evaluated against both the Power-law and Langmuir-Hinshelwood (LH) models through non-linear regression techniques implemented in MATLAB. Based on the insights obtained from the IR spectroscopy and the observed reaction mechanisms, a Langmuir-Hinshelwood model was developed to describe the catalytic behavior. The experimental data demonstrated an excellent fit to the proposed LH model, with a coefficient of determination (R^2) value of 0.99, indicating strong agreement between the model and experimental results.

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Molybdenum Carbides: An Alternative Route for Methanol Synthesis by CO₂ Hydrogenation and its Mechanistic Insights

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Abstract

This study explores the catalytic performance of iron-nickel (Fe-Ni) alloy supported on molybdenum carbides (Mo₂C) for methanol synthesis via CO₂ hydrogenation. The combination of Mo₂C with Fe-Ni offers a novel and cost-effective alternative to traditional noble metal catalysts, aiming to enhance methanol selectivity while maintaining high catalytic activity and stability. The synergistic interaction between Mo₂C and the Fe-Ni alloy is investigated, revealing that Mo₂C facilitates CO₂ activation and hydrogenation, while the Fe-Ni alloy improves hydrogen dissociation and prevents carbon deposition. Detailed mechanistic insights are provided and demonstrate that the alloy modifies the electronic structure of Mo₂C, leading to a favorable adsorption energy landscape for intermediates critical to methanol formation. Experimental results indicate that the Fe-Ni/ Mo₂C catalyst achieves superior methanol selectivity compared to conventional catalysts, with improved resistance to deactivation. This work highlights the potential of Fe-Ni alloys over Mo₂C compared to other Molybdenum suboxides and favors a sustainable and scalable solution for CO₂ utilization, offering new pathways for methanol production in the context of carbon capture and utilization (CCU) technologies

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A Zinc Single-Atom Catalyst for Efficient CO₂ Fixation into Cyclic Carbonates

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Abstract

The valorization of CO₂ into organic carbonates through its cycloaddition with epoxides has garnered significant attention in catalysis.^{1,2} However, the reaction is often hindered by low selectivities, and a key challenge is the development of catalysts capable of effectively activating both CO₂ and epoxides simultaneously.³⁻⁵ In this study, we tackled this challenge by synthesizing and characterizing a novel, bifunctional catalyst made of isolated zinc single atoms dispersed on carbon nitride. The monoatomic nature and homogeneous distribution of the zinc species were confirmed using advanced characterization methods, including X-ray absorption spectroscopy and aberration-corrected scanning transmission electron microscopy. The catalyst activity and recyclability were validated through catalytic tests with epichlorohydrin as a model epoxide, and the study was extended to also include a wide range of functionalized epoxides. Density functional theory (DFT) calculations were used to elucidate the reaction mechanism, revealing that both CO₂ and epichlorohydrin interact with the same zinc atom before cyclization, highlighting the pivotal role of zinc single atoms in facilitating the reaction. Overall, our study offers new insights into the design and optimization of heterogeneous catalysts for CO₂ cycloadditions, paving the way for more effective strategies in CO₂ conversion for the production of valuable chemicals.

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Structure, Activity and Reaction Pathway of Ni-Ru/ γ -Al₂O₃ Catalysts for CO₂ Methanation

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Abstract

In our study, we investigated the structure, activity and reaction pathway of Ni-Ru/ γ -Al₂O₃ catalysts for CO₂ methanation reaction. Here, we synthesized 'x'Ni-'y'Ru/ γ -Al₂O₃ (('x'=100,99.5,95,85)('y'=0,0.5,5,15)) catalysts by wetness impregnation method^{1,2} and deciphered their structure using XRD, HRTEM and STEM-EDX techniques and examined their CO₂ methanation performance using packed bed reactor experiments. We show that Ni and Ru in all the bimetallic catalysts are closely positioned but dispersed as individual particles on the γ -Al₂O₃ support. The packed bed experiments show an enhanced CO₂ methanation activity for all the bimetallic catalysts compared to their monometallic counterparts. The maximum CO₂ conversion of 77% was obtained at 400°C on the catalyst with 5 mol% Ru but it decreased with higher Ru loading of 15 mol%. The improved activity in Ni-Ru/ γ -Al₂O₃ catalysts can be due to the enhanced supply of dissociated hydrogen, as shown by our H₂ TPD analysis. We traced the reaction pathway using operando DRIFTS experiments. The DRIFTS analysis showed a reaction pathway via the HCOO route for both monometallic and bimetallic catalysts, but with different evolution of surface intermediate concentrations at different temperatures. A combination of the DRIFTS data with DFT simulations will be used to establish the energetically favorable CO₂ methanation pathway.

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Ni/Ce_{0.8}Zr_{0.2}O₂ Solid Solution Catalyst: A Pathway to Coke-Resistant CO₂ Reforming of Methane

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Abstract

This study highlights the importance of catalytic support and how it may be used to enhance the performance of nickel-based catalysts for use in dry reforming applications. In this study, three nickel-based catalysts—Ni/ZrO₂, Ni/CeO₂, and Ni/Ce_{0.8}Zr_{0.2}O₂ have been synthesized and their effectiveness in the dry reforming methane (DRM) reaction is evaluated. Each catalyst was thoroughly examined using a range of techniques, including XRD, TPR, BET, TPD, HR-TEM, Raman, O₂-TPD, XPS, TGA and CO₂-TPD to assess their structural and catalytic properties. Ni/Ce_{0.8}Zr_{0.2}O₂ catalyst, combining the advantages of both supports leading to solid solution, achieved the best overall performance with enhanced activity and stability. Meanwhile, Ni/ZrO₂ and Ni/CeO₂ catalyst showed a tendency towards deactivation over extended reaction times. The Ni/Ce_{0.8}Zr_{0.2}O_{2-x} catalyst demonstrated exceptional performance, achieving around 90.8% methane conversion and 91.0% CO₂ conversion at 700 °C, with the resulting H₂/CO ratio equal to one. The stability test revealed the remarkable stability against coke deposition for Ni/Ce_{0.8}Zr_{0.2}O₂. Meantime, Ni/ZrO₂ and Ni/CeO₂ are more susceptible to coke deposition, where Ni/ZrO₂ sample has more tendency towards graphitic coke deposition.

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Effect of KOH Activation on the CO₂ Adsorption-Desorption Potential in Agro-Waste Biomass

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Abstract

The amount of CO₂ in the atmosphere has been rising constantly despite adapting renewable energies. Recent development in the use of activated carbon to adsorb and sequester CO₂ has been increasingly recognized¹ as innovative approach in CO₂ sequestration. Agricultural waste biomass derived carbon constitutes an environmentally benign system for large-scale CO₂ sequestration. In this study, we report the single-step activation procedure to derive activated carbon from palmyrah kernel shell waste biomass², followed by chemical activation with KOH^{3,4} in the temperature range of 600-800 °C. The textural and chemical properties of the synthesized samples were determined using BET surface area, Fourier transform infrared spectroscopy, Raman spectroscopy, X-ray diffraction, X-ray photoelectron spectroscopy, Scanning electron microscopy, CHNS analysis, and Particle size analysis. The synthesized activated carbon showed a well-developed porous structure and an improved specific surface area of 677.95 m²/g. The sample activated at 800 °C exhibited CO₂ adsorption/desorption of 113.36/127.64 mg/g at 25 °C and 181.79/155.34 mg/g at 5 °C, both under 1 bar of pressure as assessed via the thermo-gravimetric weighing technique⁵. Thus, palmyrah kernel shell waste biomass derived activated carbon exhibit high selectivity for CO₂ adsorption over N₂, and efficient desorption of CO₂ during regeneration.

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Structural Insights into CO₂ Reduction by Formylmethanofuran Dehydrogenase

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Abstract

In this work, we have explored the enzyme activity of formylmethanofuran dehydrogenase (fmfDH), a crucial enzyme in methanogenic archaea that facilitates methanogenesis. The objective is to understand the enzyme's role in CO₂ reduction with H₂ and the structural stability of fmfDH across various methanogens¹. From our literature survey, fmfDH is identified as a key step in methane production via One Carbon Metabolism². Using Molecular Dynamic (MD) and metadynamic simulations⁴, we modeled the enzyme's structure⁵ and performance in CO₂ reduction. Through flexible docking³, enzyme-substrate complexes were generated, allowing us to test docking conformations of methanofuran and formylmethanofuran under various pH conditions.

This resulted in the identification of optimal conformers, which were subjected to i) binding energy analysis, ii) MD and metadynamic simulations to explore the reaction dynamics, iii) Gibbs free energy calculations for binding and reaction, and iv) stability assessments of the enzyme-substrate complexes. By establishing the reaction dynamics, we rank the efficiency of fmfDH from different organisms. The study seeks to understand structural adaptations within the enzyme that enhance its catalytic performance and to identify functional groups or ions that facilitate CO₂ reduction.

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Nitrogen-Enriched Mesoporous Carbon Nitride (C₃N₅) for Chemical CO₂ Fixation

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Abstract

Chemical fixation of carbon dioxide (CO₂) and epoxide into valuable cyclic carbonate is an eco-friendly pathway to utilize CO₂, and hence offer an opportunity to establish a renewable carbon economy. In this work, we fabricated nitrogen enriched mesoporous graphitic carbon nitride (mpg-C₃N₅) through template-assisted thermal polymerization process. The catalytic investigation also involved a variety of control samples such as bulk C₃N₅, potassium-doped C₃N₅, melamine, and urea-derived-C₃N₄. Solid-state NMR, EDX, XPS and CO₂ TPD analyses confirm that the triazine and triazole moieties in mpg-C₃N₅ increase the nitrogen content, resulted into low C/N ratio and high Lewis basicity. The as-synthesized and well characterized mpg-C₃N₅ catalyst demonstrated for the thermocatalytic metal/solvent-free CO₂ cycloaddition reaction in the presence of stoichiometric potassium iodide as cocatalyst. Notably, the synergism between mpg-C₃N₅ and cocatalyst enhanced the catalytic performance at atmospheric CO₂ pressure. This work demonstrates that, the adsorption, activation of CO₂ and epoxide conversion depend not only on basic nitrogen sites, but also more importantly on the surface area of mpg-C₃N₅ i.e. accessibility of basic nitrogen sites in mpg-C₃N₅. The mpg-C₃N₅ catalyst showed good scalability, reusability, and structural stability under thermal conditions. Therefore, offering a new platform for highly efficient atmospheric utilization of CO₂ to produce value-added products.

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Dry Water CO₂ Hydrates for Carbon Capture and Storage

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Abstract

Hydrate-based carbon capture and storage (HBCS) represents a sustainable and promising strategy for mitigating global warming by leveraging water, an abundant resource, to capture and store CO₂.^{1,2} However, the commercial application of HBCS faces challenges due to the inherently slow kinetics of CO₂ hydrate formation and the low conversion efficiency of water into hydrates. Dry water (DW), a water-in-air dispersion, has emerged as a potential medium to enhance CO₂ uptake and hydrate formation rates.³ Despite this, the understanding of the crystal structure, growth dynamics, and the impact of kinetic promoters in DW-CO₂ hydrate formation is still limited.^{4,5}

In this study, we present a detailed investigation of CO₂ hydrate formation in DW, addressing these challenges at both macroscopic and microscopic levels. By utilizing a combination of a custom-built high-pressure reactor, in-situ Raman spectroscopy, and powder X-ray diffraction (PXRD), we examine the crystal structure, growth dynamics, and morphology of CO₂ hydrates formed in DW, with and without the kinetic hydrate promoter L-tryptophan (Trp). Our results show that CO₂ forms structure I (sI) hydrates within DW systems, with hydrate growth observed on and beneath the silica shell. This leads to a significant increase in CO₂ uptake—approximately 2.8 times higher than in pure water (~140 v/v compared to ~50 v/v). Additionally, the incorporation of Trp in DW significantly accelerates the DW-CO₂ hydrate formation process, reducing both the induction time and the time required to reach 90% gas uptake (t_{90}) at 274.65 K. These findings provide valuable insights into CO₂ hydrate formation in DW, underscoring its potential to enhance the efficiency and scalability of HBCS technologies.

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Synergistic Catalysts for CO₂ Methanation: Synthesis, Characterization, and Mechanistic Studies of Co/NiO-MgO Nanocomposite

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Abstract

The recent scenario has witnessed a growing demand for CO₂ methanation as it is a versatile technology with the potential to address multiple challenges related to climate change, renewable energy integration, and sustainable development. Ongoing research and development efforts to optimize the efficiency and cost-effectiveness of this process for widespread adoption in the current and future energy scenarios. CO₂ methanation involves conversion of CO₂ and H₂ into methane. This chemical transformation occurs at elevated temperature and pressure, utilizing a catalyst to facilitate the reaction. In this study, a nanocomposite Co/NiO-MgO, is synthesized through sonochemical and solution combustion methods. The incorporation of Co is achieved through ionic substitution and wet impregnation technique. These methods are employed to enhance the catalytic activity of the nanocomposite. The catalysts undergo comprehensive characterization using techniques such as SEM (Scanning Electron Microscopy), XRD (X-ray Diffraction), XPS (X-ray Photoelectron Spectroscopy) and BET (Brunauer Emmett Teller). This analysis provide insights into the structural, physical properties, and specific surface area of the nanocomposites. Subsequently, the catalytic activity of these materials is assessed for the conversion of CO₂ to methane, along with an examination of methane selectivity.

Visible Light Driven Selective Production of Formate from CO₂ by Homogeneous Co-Based Molecular Catalysts in Presence of Different Additives

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Abstract

Renewable-driven, sustainable, and facile conversion of CO₂ to value added chemicals is regarded as a crucial step in CO₂ management in our ongoing fight against energy issues and mitigating the climate change crisis. In this regard, earth-abundant transition metal-based photocatalytic systems emerge as an attractive option for efficient and selective CO₂ reduction. However, designing such catalysts is an uphill task, considering their lack of activity in higher oxidation states and their inherent vulnerability in low oxidation states. In literature, there is only bimetallic Co-based molecular catalyst having bi-qpy ligand moiety which are capable for photoactivated CO₂ to HCOO⁻ depending upon the reaction condition. In this work, we have synthesized two newly developed monometallic Co(II)-based molecular catalyst having 4-aminoantipyrine moiety for visible light driven CO₂ to formate in presence of [Ru(bpy)₃]²⁺ as Photosensitizer and triethanoamine as Sacrificial electron donor in DMA medium. The reaction mechanism was explored by i) Oxidative quenching through Fluorescence spectra ii) PCET, iii) CO₂ binding. This catalyst design strategy can be expanded to produce a new genre of durable and effective CO₂-activating photocatalysts in our pursuit of reducing the carbon footprint of anthropogenic activities.

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Dual-functional Catalyst for Efficient CO₂ Conversion into Value-added Products

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Abstract

This study explores the catalytic hydrogenation of CO₂ into valuable products like methanol and dimethyl ether (DME) using a hybrid catalyst. The CFC-15 catalyst was synthesized via a hydrothermal method with a 1:1 ratio of Cu:Fe, with Ce as the remaining component. is embedded in ZSM-5 to enhance product selectivity. CFC-15 exhibits high selectivity for methanol, while ZSM-5 acts as a mesoporous shell, promoting methanol dehydration to DME. The catalytic performance is tested in a high-pressure fixed-bed reactor, with detailed characterization via XRD, FESEM, BET (133 m²/g), H₂-TPR, CO₂- and NH₃-TPD-MS, *in situ* DRIFTS, and CO₂ capture studies. A mechanistic pathway for methanol and DME formation over the CFC-15/ZSM-5 hybrid catalyst is proposed based on DRIFTS analysis. CO₂ capture studies further elucidate the relationship between CO₂ capture efficiency and the catalyst's dual functionality in promoting selective reactivity.

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Bismuth Incorporated G-C₃N₄ as an Efficient Catalyst for Light-Assisted CO₂ Fixation at Room Temperature under Atmospheric Pressure

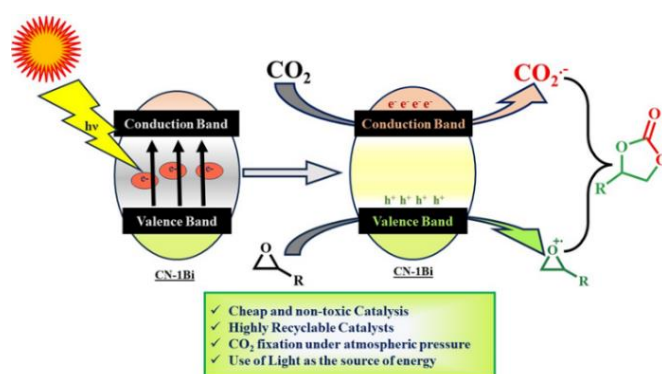
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Abstract

After the Industrial Revolution, the amount of carbon dioxide (CO₂) in the earth's atmosphere increased manifold. Since CO₂ is a greenhouse gas that causes Global Warming, the emission of CO₂ has to be controlled. Using CO₂ as a C1 feedstock industrially important cyclic carbonates chemicals can be produced in an atom-economic process.¹ Additionally, these reactions can be carried out in the presence of light energy which is a more sustainable and greener approach.^{2,3} In this work, Bi NPs doped graphitic carbon nitride (CN-xBi) material has been prepared in a simple two-step route involving calcination and hydrothermal reactions. Thorough characterization of these materials has revealed the homogeneous distribution of Bi NPs on the g-C₃N₄ sheets. Under optimized reaction parameters the active catalyst can convert a range of epoxides to their corresponding cyclic carbonates with good to moderate yield. Furthermore, the catalyst retains its catalytic activity for up to five cycles of catalysis proving its chemical stability under the operating parameters. Moreover, based on several controlled experiments and spectroscopic/electrochemical measurements a possible pathway for photocatalytic CO₂ fixation has been proposed.⁴ Overall, the study provides a convenient and sustainable strategy for CO₂ utilization under mild conditions.⁵



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Natural Kaolin Derived Ruthenium Supported Nanoporous Geopolymer: A Sustainable Catalyst for CO₂ Methanation

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Abstract

Addressing the serious concern of excessive CO₂ emission, CO₂ methanation reaction for converting environmental CO₂ to methane is a suitable way. Methane can be used not only as a fuel but also as a hydrogen carrier. In this study, the geopolymer is explored as a support which is synthesized using natural kaolin (GNK). This geopolymer support is used to disperse ruthenium (Ru) nanoparticles by a single-step hydrazine reduction method. The catalyst is characterized using various surface and bulk techniques. Further, the catalytic performance of ruthenium-supported Geopolymer (Ru/GNK) for CO₂ methanation process is explored with varying Ru % loading and with varying flow rates. Catalyst stability is also checked for 20 hours by time on stream isothermal experiment. The spent catalyst is characterized by O₂-temperature programmed oxidation (O₂-TPO) and X-ray photoelectron spectroscopy. Overall, the catalyst proved to be cost-effective and free from pretreatment requirement apart from the superior activity, high selectivity, and good stability.

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Heterostructure Nanocatalyst based on Ce-MOF and MoS₂ Towards Visible Light Driven CO₂ Reduction to Ethanol

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Abstract

The process of photocatalytic CO₂ reduction into value-added fuels and chemicals remains a highly promising avenue in the realm of renewable energy generation. However, inadequate product selectivity, low yields of multi-carbon products, and fast recombination of electron-hole pairs are the main challenges for the practical implementation of photocatalysts. In this study, we introduce a novel approach for utilizing electrostatically self-assembled Ce-MOF and MoS₂ nanosheet heterostructure, referred to as **Ce-MOF_MoS₂ NS** for catalytic conversion of CO₂ and achieved a high yield of ethanol (1947 $\mu\text{mol/g}$ in 18 hours) with remarkable selectivity of 93.6 % in water. The proximity of Ce-MOF and MoS₂ nanosheet facilitated the enhanced charge separation by creating a shorter electron transfer pathway from MoS₂ to the catalytically active low-lying 4f-orbitals of Ce⁴⁺, which has been confirmed by the transient absorption measurement, Kelvin probe force microscopy, EPR, XPS, charge density difference calculation, and photoelectrochemical measurements. The facile electron transfer from MoS₂ to Ce⁴⁺ and the existence of two CO₂ molecules near the defect site in Ce-MOF enables the C–C coupling, resulting in the formation of ethanol. Moreover, the probable mechanistic pathway for CO₂ reduction has been revealed with in situ DRIFT analysis.

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Photocatalytic CO₂ Reduction Using Mononuclear Self-Photosensitized Ruthenium Complexes: Utilization of Blue, Green, and Red Light

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Abstract

Facile conversion of CO₂ to commercially viable carbon feedstocks offers a unique way to adopt a net-zero carbon scenario. The photocatalytic reduction of carbon dioxide (CO₂) represents an attractive approach for solar-energy storage and leads to the production of renewable fuels and valuable chemicals. To date, there are numerous photocatalytic systems for CO₂ reduction based on transition metal-based complexes, which are mainly three component systems bearing a catalyst, photosensitizer, and sacrificial electron donors.¹ In this conventional system, there is a significant amount of energy loss during the transfer of electrons from activated photosensitizer to catalyst.² The integrated system where the catalyst can also act as a photosensitizer is a superior system to minimize the energy loss during ET.³ Also, to increase the effectiveness of the light absorption, a broad range of visible light absorption by the catalyst is desired.⁴ There is only very limited report for self-sensitized photocatalysts for CO₂ reduction.⁵ To further facilitate the development of panchromatic self-sensitized catalyst for CO₂ photoreduction, we developed redox non-innocent terpyridine ligand-based Ru-complexes for red light driven self-sensitized CO₂ photocatalysts which absorb with the longer-wavelength region (350–700 nm) and give exclusively carbon monoxide (CO) as CO₂ photoreduction product. A catalytic mechanism is proposed based on the detection of intermediates using various spectroscopic techniques, including transient absorption, electron paramagnetic resonance, cyclic voltammetry, and UV–vis spectroscopy.

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Exploring the Significance of CO₂ Methanation Studies on Co₃O₄ and Ni-doped Co₃O₄ Catalysts

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Abstract

The catalytic conversion of carbon dioxide to useful products such as methane is one of the best alternatives to address the growing energy demand resulting from the depletion of fossil fuels. In this work, Co₃O₄ and Ni-doped Co₃O₄ catalysts were synthesized by a single-step solution combustion method. Upto 15 atomic% Ni was successfully substituted in Co₃O₄ lattice. These catalysts were characterized by XRD, XPS, SEM, TEM, BET, ICP-OES, H₂-TPR, CO₂-TPD, CO₂-TPD-MS, CO Pulse chemisorption, and *in situ* FTIR analysis in order to know the physical, structural, morphological, elemental and redox properties of the materials. The CO₂ methanation reaction was carried out in a packed bed reactor at a GHSV of 31,800 h⁻¹ and in the temperature range of 200-450°C. The H₂: CO₂ ratio of 4:1 was maintained for all the studies to maintain the stoichiometry. All Ni-doped catalysts offered decent performance, however, the highest performance of 58%CO₂ conversion and more than 90%CH₄ selectivity was achieved without reduction, 78% CO₂ conversion and more than 98%CH₄ selectivity with reduction were obtained with 20%Ni/Co₃O₄. The apparent activation energy for 20%Ni/Co₃O₄ was 28.79±0.6 kJ. mol⁻¹.

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Tailoring 2D Ti₂CT_x MXenes Photocatalytic Systems for CO₂ Reduction: Quest for Selective Ethanol Production

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Abstract

We investigate the 2D MXene systems, specifically, Ti₂CT_x MXene, for improved photocatalytic reduction of CO₂. Employing a MILD synthesis method,¹ Ti₂C(OH)₂ MXene with -OH terminations was synthesized and characterized. Ti₂C(OH)₂ MXene being an effective electron-coupled proton donor, found to exhibit good selectivity for CO₂ reduction reactions.² The -OH functionalization has further enhanced its photocatalytic efficacy. Analysis shows the prevalence of OH terminal groups offered active sites for CO₂ reduction and facilitated the spontaneous bypassing of the activation barrier for the creation of intermediate molecules like formate and formic acid through a lower energy pathway, facilitating direct ethanol conversion (290 μmol/g_{cat}/h). DFT studies supported by free energy diagrams strongly corroborate these findings. The formation of TiO₂ nanoparticles on the MXene surface arising from self-oxidation of Ti₂C(OH)₂, plays a role in efficient charge carrier transport. Augmenting TiO₂ nanoparticles by co-precipitation has resulted in increased ethanol production (310 μmol/g_{cat}/h). This led us to further investigate the impact of abundant charge carriers in CO₂ reduction reactions (CO₂RR)³, we examined metals doped into TiO₂/ Ti₂C(OH)₂ and g-C₃N₄ 2D/2D heterojunction systems leading to a substantial enhancement in ethanol production, reaching ~780 μmol/g_{cat}/h. The favourable band alignment leading to direct C₂ formation is further discussed.

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A Novel Method to Assess Amine Solvent Degradation & Corrosivity in Post-Combustion CO₂ Capture Systems

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Abstract

Two primary challenges in post-combustion CO₂ capture using monoethanolamine (MEA) are solvent degradation and reactor corrosion [1]. The strong coordination between amines or their breakdown products with iron results in the material of construction of an amine reactor rapidly corroding. This work describes our progress in tracking amine breakdown and measuring the iron binding capacity of the solvent system to deliver a novel route for stable amine product development.

ICP-MS was used to measure the MEA-iron interaction (i.e. total soluble iron, C_{st}) by analysis of the solution in equilibrium with an in-situ formed iron hydroxide precipitate. A model was developed and successfully tested by varying the pH and MEA concentration. Amine breakdown was then mimicked in the laboratory by cycling the MEA in a single vessel through “absorption” (i.e. CO₂ capture) and “regeneration” (i.e. solvent stripping at a higher temperature). MEA breakdown (i.e. aging) was observed within a small number of cycles and the breakdown products were identified through HPLC. The binding of iron by the aged solvent was found to be higher than by the “fresh” solvent showing that the amine breakdown products are powerful corrosive agents and thereby corroborating industrial observations. The finding shows that the method can be used to further probe mechanisms of solvent breakdown, the role of iron as a breakdown catalyst and to screen novel anti-oxidants and improve amine stability.

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Experimental Investigation of CO₂ absorption and Desorption Performance Using Blended Amine Solvents

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Abstract

Most energy required for capturing CO₂ in the amine-based scrubbing process is consumed for solvent regeneration, making it too expensive for their commercial application¹. This work investigated the aqueous blends of several amines regarding CO₂ absorption-desorption performance. The total concentration was maintained at 5M and mixed with various amine molar ratios. The CO₂ absorption and desorption performances were investigated regarding CO₂ equilibrium solubility, initial absorption rate, initial desorption rate, and energy required during the regeneration process². Under the same operating conditions, the results were compared with the 5M aqueous MEA, the benchmark solvent for CO₂ capture. The results showed that the formulated blend has better desorption rates and is more energy efficient compared with conventional 5M aqueous MEA, corroborating that the formulated blend has the potential to improve CO₂ capture performance³.

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“CO₂ Activation, Utilization Using Mixed Metal Oxides” and Kinetic Study of Methanol Synthesis

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Abstract

Reliance on fossil fuels leads to rising CO₂ levels in atmosphere, resulting in severe climate change. Extensive research is being Conducted for developing suitable catalysts with enhanced CO₂ adsorption³ and activation for industrial-scale conversions as a value-added product (C1 feedstock). This Study deals with the Reaction Kinetics of methanol synthesis using prepared Catalyst carried out in a High-Pressure High Temperature Fixed Bed Reactor operating under Controlled Conditions Parameters Ranges as below Temperature (200°C -300° C)¹, Pressure (30-35 bar), GHSV (6600-8623) h⁻¹ Conditions. A Ce-Zr MMO (Mixed metal Oxides) is Prepared by the Co-Precipitation Method. The Optimum Ce/Zr ratio (supports) are crucial² for tuning the catalytic activity display much higher methanol selectivity stems from inhibition of the RWGS activity. Ce-Zr has High Oxygen Storage Capacity and other improved Properties compared to Pristine Ceria² and Pristine zirconia known by doing Characterization of Catalyst like XRD, H₂-TPR, CO₂-TPD XPS, BET Method, TEM Analysis etc., Ceria provides thermal stability, oxygen vacancies, and redox properties, making ceria flexible by doping metals, such as Zr, La., etc. The Kinetic Study is done by Relative Comparison of Industrial Catalyst and Prepared Catalyst. This Study aims to help in developing high-performance catalysts for better conversions and selectivity.

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Electrodeposited Bimetallic Copper Based Alloys as Electrocatalysts for CO₂ Reduction

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Abstract

Development of novel electro-catalytic materials based on copper metal is an economically viable and easy to scale up, due to the exceptional characteristic of copper to reduce the overpotentials. Combining Copper (active element) with other electrocatalytic metals can bring synergy in CO₂ conversion by improving selectivity and mitigating competitive hydrogen evolution reaction (HER).

In this work, electrodeposition of bimetallic alloy (Cu-Bi¹ & Cu-Sn^{2,3}) was performed on pre-treated carbon paper and evaluated for their electrochemical CO₂ conversion efficiency. Variation in morphologies and surface adhesion of the synthesized catalytic materials was obtained by varying the deposition parameters like current density, duration of plating time and bath composition. The electrodes were characterized using advanced analytical techniques like XRD, XPS and FESEM. The performance evaluation of the electrodes was studied using three electrode system. Polarization studies like CV and CA have been performed and the reaction was monitored for various products like methanol and formic acid by using NMR technique.

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Efficient Halogen-Free Bifunctional Organocatalyst for CO₂ Fixation into Cyclic Carbonates

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Abstract

Rapid industrialization exacerbates environmental issues by increasing atmospheric CO₂ concentration, leading to global warming and ecosystem disruption. A promising approach to address these issues involves utilizing anthropogenic CO₂ as a C1 feedstock to synthesize cyclic carbonates^{1,2}, which have various industrial applications, such as electrolytes in Li-ion batteries, precursors for polycarbonates and many more.³ Conventional catalytic cycloaddition of CO₂ into epoxides often relies on toxic halide anions as cocatalysts. So, the development of halide-free catalyst is highly desirable.⁴ Therefore, the current research endeavors to synthesize a novel pyrimidine-based bifunctional organocatalyst via Schiff-base condensation reaction. The synthesized catalyst was thoroughly characterized and demonstrated remarkable efficiency, converting a range of epoxides into cyclic carbonates with just 0.1 mol% catalyst loading under mild conditions (100 °C, atmospheric CO₂ pressure), without solvents or cocatalysts. To understand the catalytic process, Schiff-base derivatives with varying numbers and positions of hydroxyl groups (-OH) on the benzene ring were synthesized and tested as catalysts under optimized conditions. The studies reveal that hydroxyl groups play a critical role in activating the epoxide ring through hydrogen-bonding interactions, while imine nitrogens facilitate CO₂ activation via carbamate formation, thereby accelerating the formation of cyclic carbonates. Computational studies (DFT) confirmed these synergistic roles of hydroxyl and imine groups. Moreover, the catalyst exhibited excellent recyclability, maintaining its efficiency through six cycles. This approach presents a promising halogen-free and efficient catalytic system for CO₂ utilization.

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Electrochemical Work Function Modulation of SrTiO₃/Ti₃C₂T_x Heterostructure Towards Enhanced CO₂ reduction to Methane

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Abstract

Adverse climate effects of continuous CO₂ emissions from fossil fuel burning, depletion of fossil fuels, demand for renewable energy sources and hydrogen economy are some of the major challenges present world is facing. So, various methods and strategies have been designed to tackle this issue by reducing the CO₂ to hydrocarbons. However, these approaches are energy intensive and economically unfavourable. To this end, electrochemical CO₂ could be a sustainable approach towards mitigating continuous CO₂ emissions by transforming CO₂ to high energy density hydrocarbons. Herein, we report modulation of an electrochemical work function and the Potential of zero charge (PZC) of SrTiO₃ perovskite by its In-situ growth on the differentially functionalized (*OH and *F) Ti₃C₂ MXene towards enhanced CO₂ reduction. The electrochemical activity of these heterostructures follows the trend FMX/STO > MXOH/STO > MX/STO with Faradaic efficiency (F.E) of 66.60%, 64.14% and 60.42% for C1 products. It was established that the positive PZC and electrochemical work function follow the same trend as F.E trend for the three investigated catalysts. It is concluded that higher PZC and electrochemical work function promotes more feasible adsorption of CO₂ and enhances residual time of CO₂ intermediates promoting hydrogenation to CH₄. Furthermore, transient OCP decay method quantifies more alkaline pH at the FMX/STO-KHCO₃ interface which enhances CO₂ solubility and thus ensures higher CO₂ concentration at the interface.

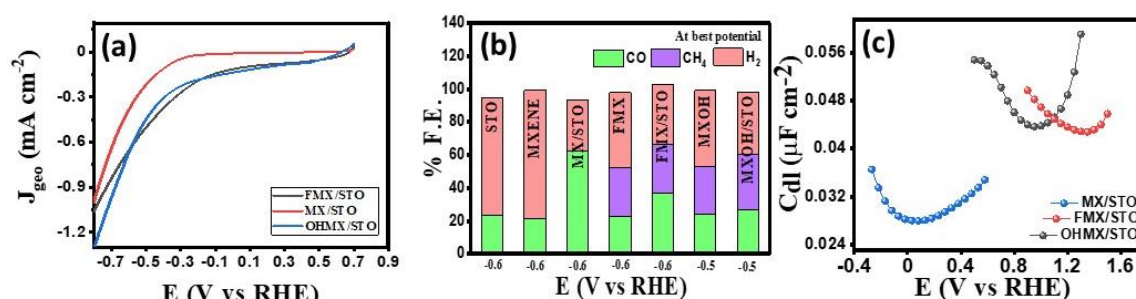


Figure 1: (a) LSV comparison, (b) catalytic activity comparison, and (c) PZC comparison for FMX/STO, MXOH/STO and MX/STO in 0.1 M KHCO₃.

Engineering Defects for Enhanced Catalytic Dry Reforming of Methane

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Abstract

Understanding the physicochemical properties of catalysts is key to establishing "structure-activity/property" relationships, which are vital for catalyst development and understanding reaction mechanisms. In this study, we investigated combustion-synthesized doped- defective fluorite $\text{La}_2\text{Ce}_2\text{O}_7$, conducting mechanistic in situ FTIR studies in the context of sustainable syngas production via dry reforming of methane. Specifically, the influence of Ni doping on B site on catalytic activity is explored. The catalysts are synthesized via single-step solution combustion synthesis. The results show that increasing the Ni concentration boosts catalytic activity by promoting active sites and enhancing coke resistance, which is linked to the presence of oxygen vacancies. The ternary doping strategy and defect engineering synergistically contribute to the catalyst's performance. This study sheds light on the design of efficient DRM catalysts and underscores the importance of nickel concentration in optimizing catalytic activity for syngas production.

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Post-Synthetic Imidation of Conjugated Porous Polymers: Enhanced CO₂ Capture and Selectivity

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Abstract

The development of porous materials for the efficient and selective capture of CO₂ is essential in addressing climate change.¹⁻³ In this study, we have presented a post-synthetic imidation strategy to synthesize robust N-functionalized porous conjugated polymers (CPPs), which includes NH-CPP, NH₂-CPP, and EDA-CPP. The synthesized CPPs contain CO₂-philic groups. Post-synthetic imidation significantly enhances CO₂ uptake, reaching 53% for NH₂-CPP and 48% for NH-CPP at 1 bar and 273 K. CO₂ uptake capacity was also assessed at higher pressures, up to 30 bar, and ambient temperature (298 K), showing a substantial increase after post-imidation, with NH₂-CPP exhibiting the highest uptake at 4.5 mmol/g. Notably, the increased CO₂ uptake results in a 200% improvement in CO₂/N₂ selectivity under typical flue gas conditions at 273 K (1 bar, 15% CO₂, 85% N₂). These results hold significant promise for potential applications in post-combustion carbon capture.

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Terahertz Conductivity of Free-Standing 3D Covalent Organic Framework Membranes Fabricated via Triple-Layer-Dual Interfacial Approach

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Abstract

Processable covalent organic framework membranes (COFMs)¹ are emerging as a potential class of semiconducting materials for device applications. Despite extensive exploration of two-dimensional (2D) COFMs, the fabrication of crystalline, self-standing three-dimensional (3D) COFMs poses significant challenges². In this work, we have developed a unique time and solvent-efficient triple-layer-dual interfacial (TLDI) approach for the simultaneous synthesis of two 3D COFMs from a single system by deliberately choosing a system of three immiscible solvents with varying specific gravities.³ The mechanical robustness of the synthesized 3D COFMs, essential for potential applications, has been assessed using the nanoindentation technique. Besides, for the first time, the optical conductivity of these free-standing 3D COFMs is analyzed using terahertz (THz) spectroscopy in transmission mode to investigate the ground state charge carrier properties. Interestingly, these membranes show excellent transmittance (>70%) at THz frequencies with very high intrinsic THz conductivities (70-100 S/m). The evaluated scattering time and plasma frequency of the free carriers of the COFMs are highly promising for future applications in optoelectronic devices in THz frequencies.

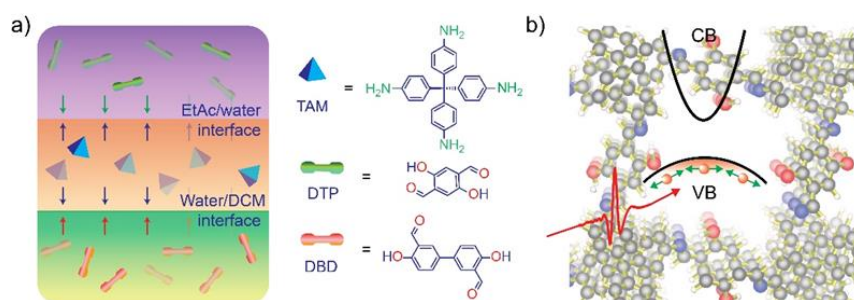


Figure 1: Schematic representation of a) TLDI approach b) intrinsic THz conductivity

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Biopolymeric Composite Membrane Blend with Mobile Carrier for CO₂/Gas Separation

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Abstract

This study investigates the preparation of a biopolymer based composite membrane for CO₂ separation application. The active layer of the composite membrane was formed by blending mobile carrier into the bio-based polymer matrix. This layer is cast onto a porous support and is responsible for the gas separation. The support provides mechanical strength to the active layer. The mobile carrier enhances the CO₂ transport across the active layer of the membrane via facilitated transport mechanism. In the facilitated transport mechanism, CO₂ reacts with amine molecules in the high-pressure region in the presence of moisture and forms an intermediate compound (carbamate or bicarbonate) which has high rate of transport as compared to CO₂ alone. The intermediate compound dissociates in the low-pressure region and releases the CO₂ molecules and regenerates the carrier. On the other hand, the non-reactive gases like N₂, H₂, and CH₄ follow solution diffusion mechanism which has low permeance compared to the facilitated transport mechanism. The inclusion of this carrier increases the selectivity of CO₂ over other gases by a significant amount as shown in Fig.1 below. Hence, higher CO₂ permeance and high CO₂/gas selectivity can be achieved.

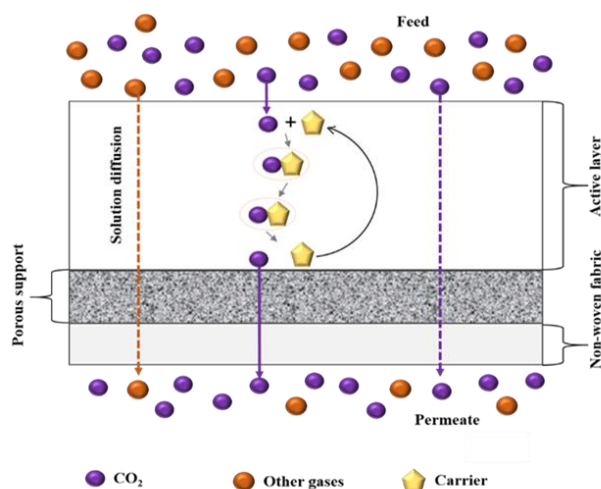


Fig.1: Schematic of facilitated transport of CO₂ using mobile carrier

Copper-Based Multi-Metallic Catalyst for Electrochemical Carbon Dioxide Reduction

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Abstract

Global warming poses a significant threat to all living organisms, with greenhouse gases—of which CO₂ constitutes 76%—being the primary contributors. To mitigate anthropogenic CO₂ levels in the atmosphere, one promising approach is the implementation of an artificial carbon cycle. The main challenges in CO₂ reduction are achieving high catalytic activity and ensuring product selectivity, with the hydrogen evolution reaction (HER) being a major competing process. The Jaramillo research group has demonstrated that benchmark copper electrocatalysts can yield up to 16 different products depending on the applied voltage. In this work, Cu-based multi-metallic metal-organic framework (MOF) electrocatalyst for CO₂ reduction was synthesized, incorporating aluminum and silver as co-metals. Benzene-1,3,5-tricarboxylic acid (BTC) was used as the organic linker. Aluminum and silver act synergistically, creating a tandem effect that tunes the copper active sites to improve product selectivity. After synthesizing MOF hydrothermally, followed by physical characterizations, including XRD, FEG-SEM, and TEM, as well as electrochemical experiments to evaluate its performance.

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Fabrication of Porous Support on Non-Woven Fabric for CO₂ Separation Applications

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Abstract

This study investigates the preparation of a highly porous polymeric support on a non-woven fabric substrate for gas separation applications. The selected polymer exhibits excellent thermal stability and chemical resistance, making it well-suited for demanding conditions involving varying temperatures and pressures. The process begins by dissolving the polymer in an appropriate solvent to create a polymer solution, which is then cast onto the non-woven fabric. This method ensures the formation of a highly porous polymer layer on the fabric, significantly enhancing the overall porosity of the support. An active layer is subsequently applied onto this porous support, which is responsible for the actual gas separation. The porous support provides mechanical strength to the active layer, while its porous structure reduces transport resistance for gas molecules during separation. Additionally, gas permeation tests assess the separation efficiency of the composite membrane. This approach offers a scalable solution for producing high-performance materials tailored for advanced gas separation technologies. The schematic of the composite membrane preparation is shown below.

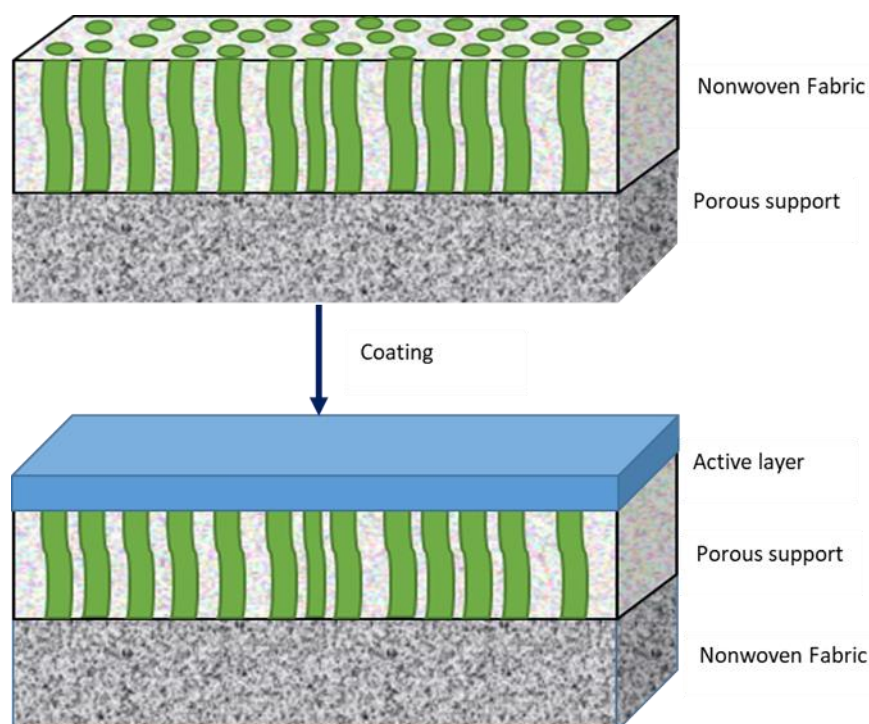


Fig. Schematic of the composite membrane synthesis

Metal Loading Effect and Comparative Analysis of Supported Monometallic Rh, Ni and Bimetallic Ni-Fe Catalysts for Efficient CO₂ Methanation

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Abstract

CO₂ methanation plays a crucial role in Power-to-Gas (PtG) technology for efficient energy storage and CO₂ mitigation^{1,2}.



This study conducts a comparative analysis of monometallic Rh/Al₂O₃, Ni/Al₂O₃, and bimetallic Ni-Fe/Al₂O₃ catalysts, focusing on the metal loading effect and reaction temperature on CO₂ conversion and CH₄ selectivity. Catalysts were synthesized using incipient wetness impregnation. Characterization techniques, including EDX, BET, H₂-TPR, XRD, and TEM, were employed to correlate catalyst properties with performance. H₂-TPR results showed that Rh/Al₂O₃ reduced at significantly lower temperatures than both Ni/Al₂O₃ and Ni-Fe/Al₂O₃, with Ni-Fe/Al₂O₃ reducing at slightly lower temperatures than Ni/Al₂O₃. XRD analysis confirmed the formation of metallic Ni and Ni-Fe alloy phases, while TEM images showed smaller particle sizes for Ni-Fe compared to Ni, with Rh exhibiting the smallest size. Methanation reactions were conducted in a packed-bed quartz reactor at 503–573 K and atmospheric pressure. The study identified the optimum metal loading as 40 wt.% for Ni/Al₂O₃ and 55 wt.% for Ni-Fe/Al₂O₃ for CO₂ methanation. For Rh/Al₂O₃, conversions increased with loading (1–12 wt%), but no optimum was reached. The optimal loadings for Ni/Al₂O₃ and Ni-Fe/Al₂O₃ are likely correlated with effective surface area of exposed metallic Ni and Ni-Fe alloy phases.

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Strain-Engineered Bismuth Oxysulfide (Bi_2SO_2) for Enhanced Electro- and Photocatalytic Performance in Water Splitting and CO_2 Reduction

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Abstract

Bismuth oxysulfide (Bi_2SO_2) is gaining attention as a versatile material for electro- and photocatalytic applications, particularly in sustainable energy processes like water splitting and CO_2 reduction. Our study explores the impact of strain on the catalytic performance of Bi_2SO_2 , aiming to enhance its efficiency for hydrogen evolution reaction (HER) and CO_2 reduction reactions (CO_2RR). By applying controlled strain, we modulate the material's electronic and excitonic properties, including its bandgap and charge carrier dynamics, leading to improved catalytic activity^{1,2}. Density functional theory (DFT) calculations reveal that strain significantly alters the adsorption energies of key intermediates, optimizing the reaction pathways for both water splitting and CO_2RR . In water splitting, strain-induced modifications in Bi_2SO_2 lead to enhanced HER by reducing the overpotentials. For CO_2 reduction, strain improves CO_2 adsorption and activation on the surface of Bi_2SO_2 ³, promoting higher selectivity toward products such as formate and formic acid. The introduction of strain not only reduces the energy barriers for catalysis but also stabilizes reaction intermediates, leading to a higher overall efficiency^{4,5}. This study focuses the potential of strain engineering in Bi_2SO_2 as a strategy to enhance its electro- and photocatalytic properties, paving the way for its application in clean energy conversion technologies.

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Unlocking CO₂ Hydrate Kinetics: Amino Acid Promoters in Industrial-Scale CCS

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Abstract

The steady rise in CO₂ emissions has sparked widespread concern about environmental and climate challenges. Researchers are now focusing on hydrate-based subsea sequestration (HBSS) in subsea sediments. However large-scale implementation of HBSS is not possible without reducing kinetics and thermodynamic barriers. Amino acids are environmentally sustainable kinetic promoters that can be used for increasing gas uptake and formation kinetics. This work has investigated the impact of amino acids (L-leucine, L-methionine) and sodium dodecyl sulfate (SDS) as kinetic promoters of the formation of CO₂ hydrates. The experiments were conducted in a continuously stirred tank reactor (CSTR) at ~275 K and 4.5 MPa injection pressure with a varying range of amino acid concentrations. The outcomes demonstrated that the kinetics of CO₂ hydrate production were affected differently by the addition of amino acids. The L-methionine structure showed a higher rate of gas uptake. The overall gas uptake (CO₂) and the hydrate conversion were not significantly affected by the amino acids or their concentrations. The experimental observation demonstrates no foam generation with amino acids as compared to SDS and a similar gas uptake profile obtained during repeated experiments. L-methionine outperforms both L-leucine and SDS as a CO₂ hydrate kinetic promoter, and it may be used in hydrate-based CO₂ sequestration technology as a kinetic promoter, which is effective, dependable, and environmentally benign.

Novel, Synergistic Oxide Catalysts: Transforming CO₂ into Carbonate(s)

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Abstract

Conversion of CO₂ into other valuable chemicals is an efficient advancement in green chemistry as well as fight against climate change. In this work, the novel, synergistic and bi-functional heterogeneous catalysts are described to convert CO₂ into organic carbonates in the aim of reducing greenhouse gas emissions and creating more valuable products at the same time. This novel catalyst, designed with highly active sites and an optimized surface structure, and an appropriate acid to basic ratio operates under mild, eco-friendly conditions, enabling the selective synthesis of carbonates with impressive yields.

This process is using CO₂, which is a greenhouse gas and the waste products are recycled to produce carbonate materials in pharmaceutical, plastic, solvent and etc. These catalysts are stable, reusable, and efficient and can easily be produced on a commercial scale.

Detailed mechanistic investigations reveal that the strong interaction between CO₂ and the catalyst's active sites drives the high efficiency and selectivity and conversion. Apart from suggesting a practical strategy of CO₂ conversion, this study also provides novel prospects for the advancements in the catalytic materials. For its potential to reduce significantly the carbon emissions, this development is expected to form part of the foundation to the new circular carbon economy.

Enhancing CO₂ Hydrate Formation Kinetics in Saline Conditions using Biodegradable Additive for CO₂ Sequestration

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Abstract

The concentration of atmospheric CO₂ has been rising sharply due to human activities, contributing to global warming and climate change. According to NASA Global Climate Change, in June 2024, CO₂ levels reached 426 ppm, marking a 20% increase since 2000. With the urgent need for CO₂ mitigation, one promising approach is the capture and storage of CO₂ in the form of gas hydrates, which occur naturally in deep-sea sediments. Gas hydrates are non-stoichiometric crystalline structures consisting of water molecules forming hydrogen-bonded cavities that can trap gases like CO₂. These hydrates remain stable under conditions of low temperature and high pressure, with the capacity to store approximately 180 m³ of CO₂ in 1 m³ of gas hydrate. The present study focuses on understanding the formation kinetics of CO₂ hydrates in silica-based sediments, particularly examining the effects of salinity. Laboratory experiments are conducted under simulated natural conditions to assess how sediment properties, such as particle size, water saturation, and porosity, influence CO₂ hydrate formation. In addition, the study evaluates the role of biodegradable additives in enhancing hydrate formation kinetics. This research aims to optimize CO₂ sequestration processes, aligning with global efforts to achieve “Net Zero” emissions targets.

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Post Synthetic Exchange in Zirconium Metal-Organic Framework for Efficient Photoreduction of CO₂ to Formate.

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Abstract

Reducing CO₂ to useful products such as formic acid is of immense industrial importance. In the present report, we have studied the CO₂ reduction performance of a Zr MOF and its Titanium-exchanged analogues. A naphthalene diimide tetracarboxylic acid (TNDI) linker-based metal-organic framework with Zirconium metal was synthesized for effective photocatalytic CO₂ reduction in aqueous medium.^{1,2} This MOF was thoroughly characterized using techniques like PXRD, TGA, N₂ BET, UV-Vis spectroscopy, and SEM. This water-stable MOF was able to achieve formate production at a rate of 38 $\mu\text{mol g}^{-1}\text{h}^{-1}$. Higher production rates and yields were achieved through the post-synthetic metal exchange of Zr with Ti.^{3,4} The new mixed metal MOF with 20% and 30% exchange of Zr with Ti metal resulted in the reduction of the band gap of the pristine MOF which led to a higher production rate of 50 $\mu\text{mol g}^{-1}\text{h}^{-1}$ and 71 $\mu\text{mol g}^{-1}\text{h}^{-1}$ of formate, respectively. Inspired by the current work, a new analogous Zr MOF has been synthesized, and characterized, and its photocatalytic activity has been thoroughly checked. This new framework is under study for its structural correlations and catalytic activity for CO₂ reduction.

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Electrochemical Co-Reduction of CO₂ and Nitrate to Urea

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Abstract

Urea is extensively used in fertilizers and is synthesized from liquid ammonia and CO₂ using the Bosch-Meiser process. The industrial production of ammonia through Haber-Bosch and subsequent urea production are highly energy intensive consuming considerable amount of fossil fuels and emits carbon dioxide gas. In contrast, electrochemical synthesis of urea from CO₂ and nitrate pollutants could offer a more sustainable process.¹ However, the electrochemical reaction is a complex 16 electron reduction reaction, involving co-activation of reactants and optimized adsorption of intermediates facilitating the C-N coupling occurring at the same site.² The challenge is to have the parallel reactions of CO₂ reduction and NO₃⁻ reduction, competing with hydrogen evolution reaction.³ In this work, Fe-Cu diatomic catalyst is used to achieve co-reduction of nitrate and CO₂ in a neutral medium at ambient conditions.

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CO₂ Electroreduction in CeO₂: Role of Doping on Oxygen Defect Formation using DFT+U Studies

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Abstract

Reducing fossil fuel dependence is key to lowering greenhouse gas emissions, and CO₂ electroreduction using renewable energy offers a promising solution. While converting CO₂ to hydrocarbons (CH_x) is energetically inefficient due to complex multielectron steps, selective CO₂ conversion to CO is more energy efficient. CeO_x-based electrodes are widely used for CO₂ electroreduction due to their mixed ionic-electronic conducting (MIEC) properties. This study investigates the effects of Pr and Gd doping on CeO₂ electrodes using DFT+U calculations.

Oxygen abstraction energies were calculated to evaluate oxygen defect formation in CeO₂ with and without Pr/Gd doping. Hydrogen incorporation into CeO₂ lowered oxygen abstraction energy, increasing Ce³⁺ formation. Bader charge analysis showed hydrogen in the CeO_x lattice occupies oxygen defect sites as hydridic species. For Pr-doped CeO₂, oxygen abstraction energies were even lower, but strong O-H bonds formed in H₂ make oxygen removal more difficult, keeping Pr-doped CeO₂ in an oxidized state. Hydrogen in the Ce {Pr}O₂ lattice was identified as protic in nature.

Adsorption studies showed CO binding energy on Ce-metal atoms was higher in Ce{M}O_x than in undoped CeO_x, suggesting an oxygen vacancy-mediated pathway involving a "metal-carbonyl" intermediate.

Methane Pyrolysis: Advancing towards Green Hydrogen Production

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Abstract

The future of energy is green, and hydrogen stands at the forefront as a clean and sustainable fuel source. Among various hydrogen production methods, methane pyrolysis offers a compelling pathway to produce hydrogen with minimal CO₂ emissions, positioning it as a vital technology for the green hydrogen revolution. This process not only provides a high yield of hydrogen but also generates solid carbon as a valuable by-product, which can be utilized in various industries.

To enhance the efficiency and scalability of methane pyrolysis, our research focuses on screening and optimizing various catalysts. By experimenting with different catalytic materials, we aim to increase methane conversion rates and maximize hydrogen output. The catalytic performance is systematically studied in a fixed-bed reactor, and the influence of key operational parameters is evaluated to ensure optimal production. This project explores innovative approaches to address the growing demand for sustainable hydrogen while minimizing environmental impacts. With ongoing advancements in catalyst technology, methane pyrolysis is set to play a critical role in shaping the future of green hydrogen, contributing to global efforts towards decarbonization and energy security and Work opens an avenue toward cost-effective and greener processes for future energy and industrial applications.

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Atmospheric Plasma Assisted Graphene Coating for Enhanced Properties of Polypropylene Fabric

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Abstract

In this study, we explore the application of atmospheric plasma-assisted chemical vapor deposition (CVD) to functionalize graphene onto polypropylene (PP) fabric, aiming to enhance its conductivity and antistatic properties¹. Polypropylene², widely used in textiles due to its lightweight and cost-effectiveness, often lacks advanced functionalities such as electrical conductivity, thermal stability, and resistance to environmental degradation due to the unavailability of functional group for bonding. By employing plasma as a surface activation agent, we effectively deposit monomer of ethylene and then uniformly coat graphene layer over the fabric by pad-dry cure and high temperature beaker dyeing, improving adhesion and ensuring homogeneity of the coating³. A stable mixture of pristine graphene was optimized using various active solvents, and the suitable solvent was identified for better adhesion and uniform dispersion over a long period of time⁴. The surface resistivity decreased from $10^{12} \Omega \text{ sq}^{-1}$ to $10^6 \Omega \text{ sq}^{-1}$ and the half decay time is less than 5 sec, indicating increased conductivity due to the direct addition of graphene onto the surface of PP. Plasma energy power, treatment duration, and concentration of graphene were optimized to achieve repeatability and stability, maintaining wash fastness⁵ for up to five home launderings under AATCC standards. This enhancement, driven by the uniform and stable graphene dispersion, opens new possibilities for polypropylene-based materials in advanced applications, including wearable electronics, smart textiles, and electrostatic discharge protection. The results underscore the effectiveness of plasma CVD in functionalizing traditional fabrics, offering a scalable and environmentally friendly approach to developing high-performance materials.

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Photoreductive Dechlorination of Chlorpyrifos using 1D Poly(Heptazine Imide) Photocatalysis

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Abstract

Chlorpyrifos (CPH) is an organophosphorus pesticide with very high national demand and consumption. This pesticide breaks down to form Trichloro pyridine-2-ol, a category-I toxic pollutant, wherein the mere presence in water is responsible for genotoxicity, motor impairment and chronic ailments. In order to abate this problem, Potassium Poly(Heptazine imide) (K-PHI), an ionic carbon nitride based photocatalytic operation was adopted for the problem with its demonstrated multielectron transfer, higher hydrogen evolution turnover, chromoselectivity and accumulation of electron in trap sites. Instead of mineralizing the toxic metabolite, photoreductive dechlorination was much more feasible and the bond dissociation energy of C-Cl (~ 52 kJ) was targeted. K-PHI was synthesized using LiCl/KCl salt melt thermal polymerization strategy. The precursors for the synthesis were varied from 4-Aminotetrazole, melamine, Dicyandiamide in different ratios to promote higher heptazine count. The heptazine count and terminal cyanamide functional groups were analysed using CHNS and C1s XPS spectra. The crystallinity of (-110) K-PHI was monitored to account for 2-dimensional cross-linking between heptazine layers. Furthermore, optical characteristics were analysed. Different concentrations of CPH and TCP were used to analyze the reaction kinetics under different visible light sources. Water as a hydrogenolysis agent was investigated to determine the mechanism of proton transfer.

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Harnessing Light-Matter Interactions with Plasmonic Copper Nanoparticles for Photothermal Studies

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Abstract

Plasmonic materials are a hub of unique optical properties such as electromagnetic field concentration, hot charge carriers, and heat, which makes them exciting candidates for light harvesting applications.¹ Photoexcited plasmonic materials can dissipate huge amount of heat into their surrounding. The study of generation, quantification and utilization of this heat is an emerging area of research in solar energy harvesting known as thermoplasmonics.² The majority of the thermoplasmonic studies are conducted with metal NPs based on Au and Ag because of their excellent chemical stability and ease of chemical synthesis.³ However, the limited availability and cost of these metal precursors have triggered the search for more sustainable alternatives to noble metal-based NPs.⁴ As a potential alternative, we have synthesized highly monodisperse and spherical-shaped oleylamine-capped CuNPs,⁵ which showed excellent long-term colloidal and compositional stability under ambient conditions. The CuNPs were ligand exchanged with charged thiolate ligands of both polarities to yield a stable dispersion of CuNPs in water. Moreover, we have addressed some of the key fundamental plasmonic and photothermal parameters of CuNPs such as photothermal conversion efficiency (~80 %) and temperature rise ($\Delta T \sim 150$ °C). Our study reveals that the CuNPs were 'hot' enough to perform high-temperature reactions such as solar-vapor generation and crystal-to-crystal phase transformation. The insight gained from this work could pave the way for establishing Cu as an affordable material for plasmon-powered processes.

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Enabling Photocatalysis Beyond the Redox Potential of Quantum Dots

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Abstract

Visible-light photocatalysis has emerged as a sustainable strategy for chemical transformations. The process of photocatalysis occurs within the thermodynamic limits set by the maximum energy of visible-light photons. This limits the range of accessible redox potentials for common visible-light active photocatalysts. Therefore, it becomes important to develop novel strategies that can drive thermodynamically challenging reactions using visible light. In this direction, recent strategies that have come up include multiphoton excitation, electrophotocatalysis etc.^{1,2} Such strategies hold a lot of potential in the context of colloidal inorganic semiconductor nanocrystals or quantum dots (QDs). QDs have been recently established as a promising class of photocatalysts because of their tunable spectral properties and redox potentials. In this work, we expand the scope and potential of QD photocatalysis by enabling thermodynamically challenging reactions using multiphoton-based processes.

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Plasmonic Ag@Cu Bimetallic Nanostructure for Hot Electron Induced CO₂ Reduction at Room Temperature

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Abstract

Traditional photocatalysts often rely on large band gap semiconductors, which confine their operation to the UV region, comprising only 3-5% of the solar spectrum [1]. Conversely, visible light-active materials, such as sulfides and selenides, face instability under reaction conditions. To overcome these limitations, researchers are exploring catalyst materials with enhanced performance and selectivity in the visible and near-infrared (NIR) regions of the solar spectrum. Plasmonic catalysis, which combines plasmonic excitation with the activation of surface-adsorbed molecules, can facilitate catalytic reactions more effectively [2]. By integrating plasmonic metals with traditional catalytic metals, both light conversion and molecular adsorption are improved, expanding the scope for photocatalytic reactions with greater efficiency and selectivity [3,4]. In this study, silver-copper bimetallic plasmonic nanoparticles of varying shapes, sizes, and compositions were synthesized and thoroughly characterized optically and structurally. These catalysts were employed for the photo-chemical reduction of CO₂ to value-added chemicals at ambient temperature. A proposed reaction pathway for the plasmonic CO₂ reduction reaction (CO₂RR) with this bimetallic catalyst system is also presented.

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Agro-Industry Waste Derived Akermanite Nanoparticles as Photo Catalyst for Industrial Waste Water Purification

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Abstract

Water pollution has become one major environmental issue due to the rapid growth of industrial sector as they dispose the wastewater directly to the water bodies. The wastewater contains various heavy metal ions and organic dyes which need to be treated before exposure to the environment. The present study reports the facile synthesis of akermanite nanoparticles from agro-industry waste rice husk ash and ground granulated blast furnace slag by hydrothermal method. The prepared product was investigated by X-ray diffractometry, field emission scanning electron microscopy, UV-visible and fourier transform infrared spectroscopy characterization techniques. XRD and FTIR revealed the prepared powder is akermanite and the standard crystallite size was determined. FESEM demonstrates the morphology of the material and bandgap was analysed using diffuse reflectance spectroscopy. The photocatalytic activity of akermanite nanoparticles was studied using standard methylene blue dye. The effect of initial dye concentrations, catalyst dosage on the degradation of methylene blue were evaluated under visible light irradiation.

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Highly Efficient Photocatalytic Hydrogen Generation Using Water-Stable Low-Dimensional Metal Halide Perovskites

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Abstract

In recent years, the development of lower dimensional perovskites (LDPs) has shown immense promise in their structural stability against moisture. However, they still degrade quickly when exposed to a beaker full of water and lack the efficient charge carrier transport compared to their 3D bulk counterparts. This inhibits their pertinence in the solar to fuel conversion applications. Herein, we have synthesized the LDP halides, viz. (4,4'-VDP)Pb₂X₆ (X = Br, I) which are structurally 1D, by employing the idea of combining pi-conjugation and cation-pi interactions. The pi-conjugated spacer cation connects electronically the inorganic layers which is manifested in the photoconductivity enhancement across the sample. Whereas the strong intermolecular cation-pi interactions, possible via the optimal stacking of pi-conjugated spacer, are responsible for excellent moisture stability. Both the (4,4'-VDP)Pb₂X₆ halides demonstrated exceptional structural and photo- stability in water and (4,4'-VDP)Pb₂I₆ has been synthesized and characterized for the first time in this work. Moreover, we have investigated the applicability of (4,4'-VDP)Pb₂X₆ perovskites as photocatalysts, in the aqueous HX medium, to generate photocatalytic hydrogen. Remarkably, (4,4'-VDP)Pb₂I₆ has shown substantial H₂ yield in the aqueous HI medium compared to the some of the archetypical 3D perovskite, viz. MAPbI₃. The amount of H₂ generated at the end of photoreaction time of 24 h was about 1812 μmol/g. Besides, the photocatalytic H₂ generation from (4,4'-VDP)Pb₂I₆ perovskite has been performed without the use of any co-catalysts like Au, Pt, etc. Further, the (4,4'-VDP)Pb₂Br₆ does not exhibit any photocatalytic H₂ evolution in the aqueous HBr medium.

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Enhancement of visible light photocatalytic activity of g-C₃N₄ by tuning bandgap and morphology

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Abstract

With the progression of civilizations, the search for more efficient fuels has always been ongoing, and now hydrogen is at the forefront due to its high utilization efficiency. Graphitic carbon nitride (g-C₃N₄) has emerged as a promising photocatalyst for the production of green hydrogen via photocatalysis. However, its potential in visible light photocatalysis is hindered by its wide band gap. In this study, we employ bandgap engineering to fine-tune the g-C₃N₄ band gap, enabling the absorption of lower energy photons and expanding its effectiveness. The morphological modifications of g-C₃N₄ are synthesized through thermal exfoliation and hydrothermal methods. The catalysts are modified by 1 % Rhodium doping to boost its activity. XRD, XPS, SEM, DRS, UPS, PL, TCSPC, NMR, ESR, and BET are used to characterize the catalysts. Hydrogen evolution experiments are conducted with Na₂S and Na₂SO₃ as hole scavengers under a solar simulator, while DFT studies using BURAI optimize the catalyst structure. The results reveal a striking 14.3-fold increase in photocatalytic activity and a 43.2% apparent quantum efficiency due to Rhodium doping, introducing a novel approach to enhance the efficiency of g-C₃N₄ in photocatalytic water splitting. These findings hold significant potential for advancing sustainable green hydrogen production.

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Bimetallic Copper and Zinc Single-Atoms Decorated on Graphitic Carbon Nitride for Photocatalytic Carbon Dioxide Reduction to Methanol

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Abstract

Nowadays, societies are facing the biggest problems in energy requirements and the rise in CO₂ gas emissions. The conversion of CO₂ gas into value-added chemicals of higher value, including ethanol, methanol, and formic acid, is one of the main problems scientists are now confronting.^{1, 2} Methanol is one of these necessary fuels that work well in various ways.² This study uses a straightforward calcination procedure to create bimetallic Cu-Zn single atoms decorated on g-C₃N₄ support (Cu-Zn@g-C₃N₄) photocatalyst.³ The as-prepared g-C₃N₄ bi-metallic single-atom catalysts (SACs) material was characterized using various analytical and spectroscopic techniques. The material was discovered to have low metal loading of Cu and Zn metal, thin, among other intriguing features. Cu-Zn@g-C₃N₄ encourages a high CO₂ conversion, which results in a product yield of methanol that is selectively high (>4700 μmol g⁻¹). The straightforward synthesis process for the g-C₃N₄-bimetallic SACs and their use in the photocatalytic conversion of CO₂ to methanol was described in this work.

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α -C(sp³)-H (Hetero)Arylation of Thioethers Enabled by Photoexcited Triplet Ketone Catalysis

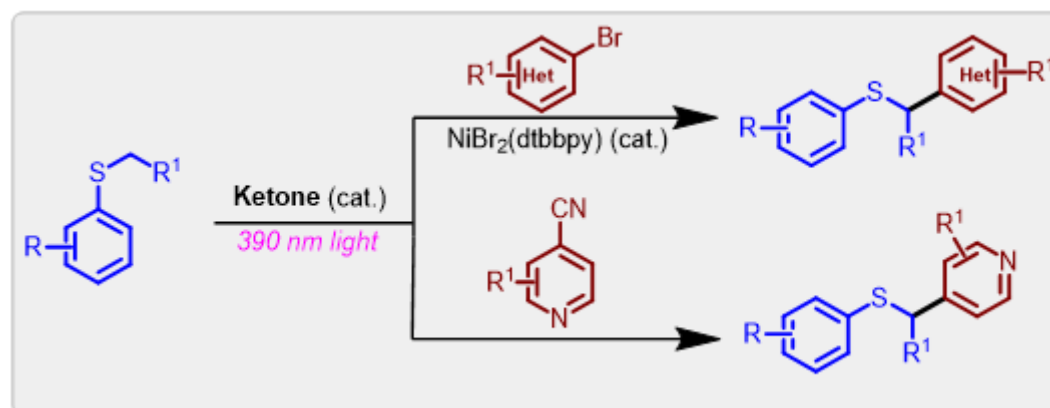
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Abstract

We report herein, α -C(sp³)-H (hetero)arylation of thioethers enabled by dual nickel and photo-excited triplet ketone catalysis. The mild reaction conditions of this protocol tolerate a variety of functional groups and further facilitate the late-stage functionalization of biologically relevant molecules to afford corresponding products in moderate to good yields. Preliminary mechanistic studies suggest that the generation of α -thioalkyl radical takes place through a hydrogen atom transfer (HAT) event, which is involved in the rate-limiting step. Furthermore, we also report the successful execution of photo-excited triplet ketone catalysed radical-radical coupling between thioanisole and 4-cyanopyridine.



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Photocatalytic Nitrogen Fixation of Oxygen Vacancy Enabled Pd-TiO₂

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Abstract

In this work, we have synthesized Pd doped anatase TiO₂ by a simple sol-gel method to introduce oxygen vacancies and Pd sites on TiO₂, where Pd is photo-deposited on anatase TiO₂. The oxygen vacancy (V_o) enhances the adsorption of N₂ on the catalyst surface. The Pd doping induced a defect energy level below the conduction band, which prefers to accept the photogenerated electron. V_o captured electron tends to move to the adsorbed N₂ and activate it. Pd sites, on the other hand, is a H₂ production center. It supplies enough H₂ so that N₂ can be hydrogenated to generate NH₃. Pd-doped TiO₂ exhibits a high NH₃ production rate of 90.50 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$, which is almost six times higher than that of pure TiO₂. This manuscript offers a possible way to create a very effective photocatalyst to produce NH₃.

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Emergence of Sustainable Sulfur nanomaterials for Efficient Solar to Energy Conversion

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Abstract

Sulfur nanomaterials are recently developed sustainable luminescent materials with several advantages. Herein, we have synthesized luminescent S dots in a cost-effective synthetic route and further modified by a slow growth process using solvent extraction phenomena. Their morphology, elemental, and optical properties have been critically investigated. The modified S dots possess better crystallinity with a higher extent of molecular sulfur, resulting in increased visible light absorption cross-section and improved charge separation followed by free carrier accumulation on desired active sites for photocatalysis. While normal S dots show polycrystallinity with a lesser extent of molecular sulfur. Finally, both the S dots have been utilized for the photocatalytic coupling reactions of benzylamine at complete ambient conditions by utilizing photoinduced electrons and holes. Further, a 2D multilayer S- sheet was synthesized from S- S- nanomaterials having high molecular sulfur content with highly defined structure. That is further used for photocatalytic azo coupling. The photocatalytic mechanisms were crucially investigated by tracking the photo-induced free radicals and intermediates. Finally, this indicates a new direction for an easier, greener, and more affordable way for specific chemical reactions.

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Au-MoS₂ Quantum Dot Composites: Structural Modification for Enhanced Catalytic Efficiency in p-Nitrophenol Reduction

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Abstract

The world's most pressing challenges now are rising human energy use and the resulting environmental damage. Photocatalysis, which utilizes light and a catalyst to accelerate a chemical reaction, is one of the most promising new forms of catalysis. Semiconductor compounds used as catalysts in the physicochemical process of photocatalysis show promise for removing dangerous environmental pollutants. A transition metal doping approach was developed to change the physicochemical properties of semiconductors, decreasing band gaps and generating barriers for free charge carriers, hence enhancing semiconductor photocatalysis efficiency. Two gold nanoparticle composites, a gold nanorod-molybdenum disulfide quantum dots, and a gold nanosphere-molybdenum disulfide quantum dots that are architecturally distinct were prepared and reduced p-nitrophenol using a reducing agent, sodium borohydride (NaBH₄), in the aqueous medium. TEM, XRD, FTIR, SEM, and other methods were used to characterize the properties of these catalysts. The crystalline structure of the produced catalysts prior to and following the reaction was also investigated. Physical-chemical characteristics, including apparent rate constant (k), were examined for each system. As a result, this study focuses on understanding the structural role of AuNR-MoS₂ QDs and AuNS-MoS₂ QDs composites, which is critical in determining catalytic efficiencies as evidenced in the reduction of aromatic nitro compounds.

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Ag Nps Modified $\text{Ag}_3\text{AsO}_4/\text{g-C}_3\text{N}_4$ Hybrid for Effective Photocatalytic Removal of 4-Chlorophenol under Visible Light

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Abstract

The $\text{Ag}_3\text{AsO}_4/\text{g-C}_3\text{N}_4$ (AA/gCN) hybrid, incorporating Ag nanoparticles (NPs)¹, was synthesized via an electrostatically driven assembly method² by combining Ag_3AsO_4 with graphitic nitride. Comprehensive characterization involved analyses of phase structure, morphology, and optical properties using X-ray diffraction, FTIR, SEM, TEM, UV-vis DRS and PL spectroscopy, along with XPS for insights into chemical composition and surface properties. The AA/gCN hybrid exhibited superior photocatalytic performance attributed to enhanced light absorption, efficient charge separation and enhanced charge transfer. The optimal AA/gCN hybrid demonstrated remarkable degradation efficiencies, achieving 76% for 4-chlorophenol under visible light irradiation within 150 minutes. Catalytic investigations were monitored using UV-vis spectroscopy and HPLC-PDA techniques. The radical trapping experiments suggested the predominant involvement of superoxide radicals ($\text{O}_2^{\bullet-}$) and holes (h^+). These findings highlight the promising potential of the AA/gCN hybrid for applications in environmental remediation and emphasizing its pivotal role in tackling modern environmental challenges.

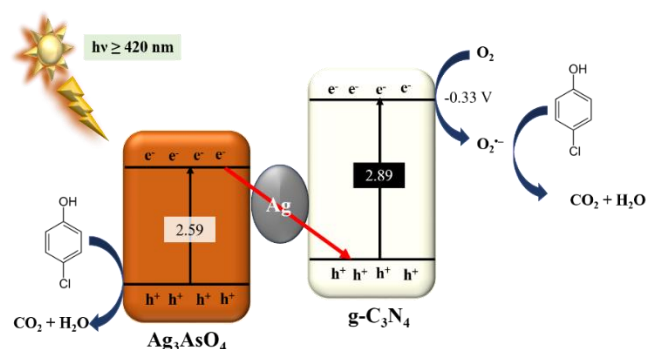


Figure 1. Schematic Representation of the Photocatalytic Mechanism

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Metalloporphyrin based Solar Photocatalytic Degradation of Lignin

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Abstract

The abundant aromatic lignin produced from agricultural biomass can serve as a sustainable alternative for various platform chemicals and fuels. However, its highly cross-linked and randomly polymerized structure poses challenges for valorization. In this study, we developed a solar photocatalytic system using porphyrins that can directly depolymerize lignin and lignin model compounds. We evaluated the porphyrins for their photophysical properties, including singlet oxygen and fluorescence quantum yields. The catalyst was initially tested on lignin model compounds before applying it directly to lignin. To assess the degraded lignin, we employed various characterization techniques such as UV–Vis spectroscopy, heteronuclear single quantum coherence spectroscopy (HSQC), electron paramagnetic resonance (EPR), mass spectroscopy, and gel permeation chromatography (GPC). A plausible mechanism for the breakdown of lignin and its model compounds was proposed after investigating the photocatalytic system under different experimental conditions. We also evaluated the recovery and recyclability of the photocatalyst. This solar-assisted photocatalytic process for lignin valorization, driven by light-harvesting materials, represents a smart and sustainable approach to simultaneously address agricultural waste and generate valuable platform chemicals.

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Selenium-Loaded Bi₂WO₆/g-C₃N₄ Hydrogels for Tetracycline Degradation with Visible Light-Activated Peroxymonosulfate

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Abstract

The post-COVID-19 era has intensified health and environmental concerns due to the uncontrolled discharge of pharmaceuticals and antibiotics. Consequently, intensive efforts are required to develop sustainable technologies at both fundamental and applied levels to address the threat of emerging contaminants [1]. Photocatalytic activation of Peroxymonosulfate (PMS) has emerged as a promising technology among advanced oxidation processes (AOP) for solving the problem of antibiotic pollution [2].

In this study, a binary photocatalyst Bi₂WO₆ (BWO) and graphitic C₃N₄ (GCN) has been synthesized using hydrothermal route [3]. While this strategy overcomes the rapid recombination of redox charge carriers, it often neglects the photocatalyst's recovery and reusability [4]. Therefore, to overcome the problem associated with BWO-GCN we designed Se-loaded BWO-GCN hydrogels using Carboxymethyl Cellulose (CMC) solution [5]. The performance of the prepared photocatalysts for tetracycline antibiotics were measured in a photocatalytic reactor set-up under visible light illumination along with aeration. The catalysts achieved a remarkable 91% degradation efficiency for 10 ppm in 30 minutes and maintained stability for up to 7 cycles, with activity decreasing to 72% after the 7th cycle. The advantages of the catalysts, which enhance the reaction, were evaluated using several characterization techniques, including XRD, FTIR, SEM, XPS, UV-DRS, and EIS. Thus, this work highlights a rational approach to sustainably enhance the effectiveness of photocatalysis technology.

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Self-Assembly of Plasmonic Nanoparticles upon Interaction with Amino Acids

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Abstract

Amino acids are essential building blocks of proteins, which are vital macromolecules with diverse functions in biological systems. Understanding and utilizing the interactions between nanomaterials and amino acids has significant potential in fields like nanomedicine, materials science, and nanotechnology. This study investigates the interactions of plasmonic nanoparticles, specifically gold (Au) and silver (Ag) nanoparticles, with amino acids. It was found that these nanoparticles form linear assemblies exclusively with certain amino acids: Au nanoparticles assemble with cysteine, while Ag nanoparticles form similar structures with methionine and aspartic acid. These interactions were analyzed using various techniques such as UV-visible spectroscopy, Fourier-transform infrared spectroscopy (FTIR), dynamic light scattering (DLS), transmission electron microscopy (TEM), and isothermal titration calorimetry (ITC). Finite-Difference Time-Domain (FDTD) simulations were conducted to model the electric field intensity of the nanoparticles during their interaction with amino acids. The paper also proposes a possible mechanism for the nanoparticle chain-like assembly with specific amino acids. This research enhances the understanding of nano-bio interfaces, with broad applications in technological fields.

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At Circumneutral Ph Photocatalytic Activity of P-Nitrophenol by Starch Composite Mo Doped Iron Pyrite Nanoparticles

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Abstract

In the Fenton reaction, there are some critical limitations like acidic pH requirement, Fe^{3+} to Fe^{2+} reverse reaction slow step, and high amount use of H_2O_2 . To overcome these problems iron pyrite nanomaterial is used. But in iron pyrite, the S-S bond undergoes breakdown and generates sulfate. To resolve this problem iron pyrite-formed composite with starch. The solvothermal method was used for the synthesis of the composite. In the iron pyrite, Mo was doped to increase its catalytic activity. The starch and the dopant were functionalized on the surface of the pyrite to prevent the leaching of iron. The catalytic nanocomposite is St/FS-x which degrades an organic pollutant present in wastewater under optimized conditions of neutral pH, cool white LED light, and lower concentration of hydrogen peroxide (H_2O_2). The St/FS-4 shows the best photo-Fenton activity towards PNP degradation. The turnover frequency (TOF) of the St/FS-4 composite was $532.87 \mu\text{molg}^{-1}\text{min}^{-1}$. Hydroxyl radical is the main active species during the Fenton and photo-Fenton reactions. The catalytic nanocomposite exhibits photo-Fenton catalytic efficiency ranging from 100-95% and recyclability ranging from 1-4 cycles.

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Photocatalytic Water Splitting by WO_{3-x}/g-C₃N₄ Heterostructure Nanocomposites for Green Hydrogen Production

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Abstract

Photocatalytic solar water splitting without a sacrificial agent has been recognized as a promising strategy for producing green hydrogen. Recently, two-dimensional (2D) g-C₃N₄ has garnered significant attention for its potential in visible-light-driven hydrogen generation. Non-stoichiometric tungsten oxide, synthesized using air thermal plasma, is incorporated into polymeric g-C₃N₄ frameworks to create a heterojunction that improves charge separation and transport. The nanocomposites were synthesized by ultrasonication process, followed by thermal treatment. The structural, optical, and morphological characteristics of the nanostructured composites have been analyzed using various techniques, including X-ray diffraction (XRD), FT-IR, UV–Vis spectroscopy, BET surface area analysis, high-resolution transmission electron microscopy (HR-TEM), X-ray photoelectron spectroscopy (XPS), and photoluminescence (PL) spectroscopy. The synthesized hybrids, functioning as visible-light-sensitive photocatalysts, demonstrated remarkable efficiency of hydrogen production *via* solar water splitting. The enhanced photocatalytic activity of the optimised photocatalyst is attributed to the synergistic mechanisms resulting from an increased specific surface area, a greater number of reactive sites, improved light absorption, and enhanced separation of photogenerated carriers.

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Effect of Aqueous DES as Reaction Media for Photocatalysed Amine Oxidation

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Abstract

The amine to imine transformation is important because imines are primarily used as intermediates in various organic synthesis within the pharmaceutical industry. The effect of aqueous media on the visible light induced aerobic oxidation of amines using TiO_2 -TEMPO (2,2,6,6-Tetramethylpiperidine-N-oxyl) and dye-sensitized TiO_2 -TEMPO coupled photocatalytic system were studied. The amine oxidation reaction was conducted in different aqueous mixtures of various deep eutectic solvents (DES) under light irradiation. An increasing water fraction in the TiO_2 -TEMPO catalyst system resulted in a significant decrease in the conversion of amine. These results highlight the potential of dye-sensitized TiO_2 system to overcome the limitations posed by water in photocatalytic processes.

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Nanoscale Energy Balance of Plasmonic Antenna-Reactor Catalyst for Light Driven Reactions: Role of Hot Carriers vs. Photothermal Effect

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Abstract

Light driven plasmonic-catalysis is seen as a potential alternative to traditional thermal catalysis. Plasmonic nanostructures in plasmonic catalytic systems act as excellent light harvesters,^[1] driving reactions forward by a combined influence of hot-carrier mediated activity and photothermal effect. Further, the tunability of the light-matter interactions in plasmonic nanostructures through compositional^[1] and structural variation^[2] ^[3] ^[4] is an added advantage for their application under different conditions.

In plasmonic catalysis, the relative contribution of hot carriers and the photothermal effect is a matter of much debate. Adopting the antenna-reactor system for analysis, this work presents the nanoscale energy balance of a Au-Pt nanoparticle system to dissect this mechanistic aspect, as well as to reveal the key factors influencing the experimental results^[5]. Based on existing benchmark experimental data⁴, the analysis shows that utilization of <1% of absorbed energy for hot carrier driven activity, resulting in a 4-fold enhancement in the rate constant of plasmon-enhanced dehydrogenation. For the disentanglement of thermal effects, a very high light intensity (>10 sun intensity for 4 cm² films) or system size (>144 cm² film for 1 sun intensity) is required to attain accurately measurable temperatures. Analysis of different nano-configurations demonstrates the clear merit of the antenna-reactor photocatalyst design.

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Nanomaterials and Biomass-Based Composite Membrane for Water Treatment Application

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Abstract

Polymeric membranes have shown great potential for the separation processes for water treatment applications. Developing sustainable and efficient materials for water treatment applications has attracted significant attention from researchers. Using several synthetic polymers creates waste and shows a major fouling problem for the membrane itself. The use of nanomaterials like SBA-15, and TiO₂ enhances the use of biopolymers for water treatment applications using separation technology. In this study biomass derived from natural waste material and highly porous nanomaterials are selected for the water treatment application. This derived cellulose acetate (Cac) biopolymer worked as the polymeric backbone of the membrane. The porous nanomaterials SBA-15 provide structural changes to the membrane matrix. The incorporation of nanomaterials TiO₂ is for photo catalytic activity. The composite membrane material shows enhanced structural, morphological, and functional properties. XRD, FTIR, FESEM, and EDS techniques used to characterize the materials and the membrane performance and efficacy evaluated by water flux determination. The pure water flux of 1818 L m⁻² h⁻¹ was achieved with biopolymer and SBA-15-based membrane showing high oil removal efficiency of more than 97%. The photocatalytic activity of the material was also studied using UV-VIS spectroscopy result with good activity with TiO₂. The developed membrane can be used effectively for wastewater treatment with enhanced flux, antifouling properties, and photocatalytic activity.

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Metal Organic Frameworks Decorated Polypyrrole Nanorod as Super-Adsorbent Towards Pollutants in Continuous Flow

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Abstract

Environmental pollution due to contaminant water poses serious concern to human health & ecosystem¹. Metal Organic Frameworks (MOFs) are known to be potential adsorbent of pollutants². They have very rich porosity, high crystallinity. But due to its stability concern in acidic & basic media, they are often ignored in wastewater treatment. In this work, we have decorated series of MOFs on Polypyrrole nano rods to enhance stability as well as adsorption ability. This material can work in a broader pH range. To check its adsorption ability, we have taken cationic, anionic dyes as pollutants along with industrial pollutants. We have compared the adsorption ability of dyes & industrial waste in both batch & continuous flow using packed bed reactor. Continuous Flow adsorption gives 10 folds faster adsorption of dyes than batch adsorption. Also, this shows excellent reusability. Thus, by incorporating composite with MOFs as well as introducing flow process in to adsorption, this material can be potential purifier of water.

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Carbon Sequestration and Structural Changes in Soil-Based Alkali Activated Binders

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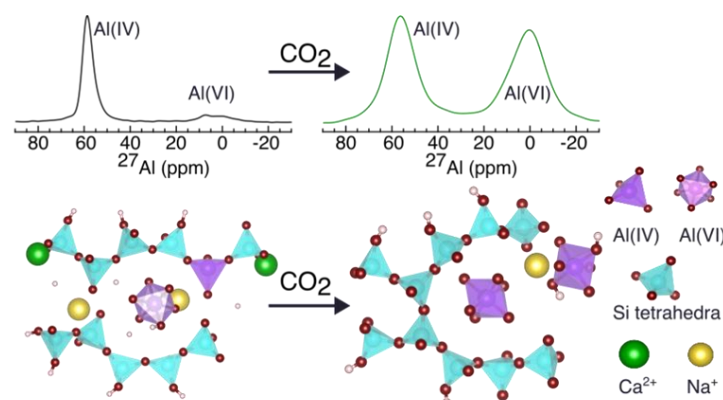
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Abstract

Alkali activated binders (AABs) are low carbon footprint alternatives to the ordinary Portland cement (OPC). Accelerated carbonation can further mitigate the CO₂ emission while enhancing the binding properties of AABs and sequestering CO₂. We used solid-state nuclear magnetic resonance (NMR) in combination with XRD, IR and DFT calculations to track local structural changes as a function of material precursors, and carbonation to unravel CO₂ sequestration mechanism and its impact on the binding properties. We report a carbonation induced Al(IV)-Al(VI) conversion together with increased branching and disorder in soil containing AABs using ²⁷Al and ²⁹Si NMR. To gain insight into the CO₂ sequestration mechanism and its impact on the binding properties, we performed multinuclear ²³Na, ²⁷Al, ²⁹Si, ⁴³Ca and ¹H solid-state NMR along with 2D correlation NMR experiments.



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Multicomponent Heterojunction Photocatalyst NGT/G-C₃N₄/BiOBr_{0.75}I_{0.25} for UV-Visible-NIR Responsive Photocatalytic Degradation of Rhodamine B

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Abstract

A wide solar spectral range responsive multicomponent heterostructure photocatalyst NGT/g-C₃N₄/BiOBr_{0.75}I_{0.25} was successfully synthesized and used for the UV-visible-NIR photodegradation of the dye Rhodamine B [1][2]. Our study shows that heterostructure overcomes the drawbacks of limited visible-light absorption and fast charge recombination of g-C₃N₄. Herein, BiOBr_{0.75}I_{0.25} extends the absorption in visible region and endorses the separation rate of photogenerated charge carriers [3][4]. Upconversion nanoparticles NaGdF₄: Tm/Yb (NGT) absorbs the infrared light and emits at 450 nm and 475 nm, which overlaps with the absorption range of g-C₃N₄/BiOBr_{0.75}I_{0.25} nanocomposite. Thus, NGT further facilitates the photocatalytic activity of the heterostructure [5]. Extensive structural, morphological, and compositional analysis was done using XRD, TEM-EDAX, XPS, and FTIR measurements. UV-visible absorption, PL emission, time-resolved decay, and electrochemical impedance spectroscopy were used to probe the separation rate of photogenerated electron-hole pairs and efficient energy transfer in NGT/g-C₃N₄/BiOBr_{0.75}I_{0.25} heterostructured nanocomposite. The photodegradation efficiency of the heterojunction was 98%, which is much higher than the bare g-C₃N₄ (74%). The heterostructure showed long-term reusability, photodegradation efficiency 97.02% even after four consecutive degradation cycles, and makes it a preferable material for photocatalytic dye degradation.

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Simultaneous Degradation of Cr(VI) and Methylene Blue by PEG Modified Manganese Ferrite (MnFe₂O₄) : Nanoadsorbent and Photocatalyst

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Abstract

Manganese ferrite (MF) and PEG modified MF (PEG-MF) NPs were prepared by using co-precipitation method¹. These NPs were used for the removal of hexavalent chromium by adsorption, and also of methylene blue (MB) dye by photodegradation in aqueous medium. About 79 % of Cr (VI) was adsorbed on 0.2g/L PEG-MF NPs in 40 mL of 1 ppm K₂Cr₂O₇ solution. The adsorption capacity was about 34.6 mg of Cr (VI) per g of adsorbent. The adsorption was found to follow Langmuir isotherm as well as pseudo-second order adsorption model². The maximum adsorption occurred at pH 8. Thermodynamically, the adsorption of Cr(VI) was found to be endothermic and spontaneous³. 83% was the highest desorption percentage which was observed in the study using NaOH. Decolouration through photocatalytic degradation of MB occurred in aqueous medium under UV irradiation⁴. Photodegradation was more effective in MF NPs than PEG-MF NPs. The current study inferred that PEG-MF NPs are magnetic nanoadsorbents/ photocatalyst which are cost-effective, easily separable and enabled efficient for the removal of various wastewater contaminants.

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Blue-LED-Driven Green Chemistry: Pioneering Sustainable Strategies for C-X Bond Formation

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Abstract

In this work, we have developed a facile, scalable, metal-free, blue LED-driven greener pathway for the efficient construction of novel C-X bonds, tackling a significant challenge in modern synthetic chemistry. The development of C-X bonds, particularly C-N and C-P, has garnered tremendous interest due to their versatile applications. Our approach leverages metal-free photoredox catalysis, a key strategy in advancing green chemistry. Specifically, we explored innovative photoredox-mediated synthesis routes to achieve the formation of guanidine from thiourea and amines *via* desulfurization, as well as the synthesis of phosphine thioamide using phosphine oxide and dithiocarbamic acid. The structural integrity of synthesized products was confirmed and characterized through NMR, HRMS, and single-crystal XRD, showcasing the efficiency and practicality of this green synthetic approach.

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The Magic of Morphology: A TiO₂ Story

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Abstract

Anatase phase of TiO₂ has been widely studied due to its extensive industrial applications [1], [2]. Here we present a novel, economically feasible and simplistic wet chemistry approach to synthesize titania crystals with high index facets with particle size control over 3 orders of magnitude (5 nm-3000 nm). Herein, unique structures were generated such as coral -shaped structure, which provides high surface area while faceted crystals formed serve as host for active metal sites. Further, we have also explored the crystallization pathways of anatase crystals. These uncontrolled pathways were intervened using modifiers (organic molecules and inorganic salts) to generate more desired faceted crystals. The as synthesized anatase agglomerates were evaluated for their photocatalytic performance. The particles with faceted morphology and a novel architecture having corrugated surface exhibited highest dye degradation efficiency of 65% which was even higher than degradation efficiency of the commercial anatase crystals (~40%). It is evident from these results that the morphology of particles plays a decisive role in determining their catalytic performance. A complete blueprint will be presented for rational design of titania crystals. Here, we controlled three aspects of particle physiology: (i) size, (ii) dimensionality, and (iii) morphology. Titania is a multifunctional material with substantial industrial applications and therefore a facile synthetic strategy to produce particles with varying morphology becomes essential.

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One-Pot Photoreforming of Polylactic Acid Waste to Valuable Chemicals

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Abstract

Since 1950, more than 8 billion tons of plastic have been produced, making polymers one of the most commonly used and discarded materials in our day today life. Unlike traditional petroleum-based plastics, polylactic acid (PLA), the most common biodegradable plastic, can break down into carbon dioxide and water in the environment. However, this natural degradation cost a significant amount of time and releases carbon in the process. Thus, there is a urgent need for development of new transformation methods that can upcycle plastic waste into valuable products, particularly with a focus on high chemical selectivity. Ambient-temperature photo-reforming provides an easy and energy-efficient method for converting PLA into value-added products. In this work, we have developed graphitic carbon nitride (g-C₃N₄) based nanocomposite material for photoreforming of real-world PLA waste into alanine and other valuable chemicals. The chemical composition and light absorption properties of g-C₃N₄ significantly influence its photocatalytic performance. However, g-C₃N₄ faces limitations, such as a high recombination rate, which reduces its photocatalytic efficiency. To address this issue, incorporating cocatalysts can improve its electrical conductivity and charge transfer capacity, which ultimately enhancing its photocatalytic activity. Thus, effective strategies that combine depolymerization and the upcycling of real-world PLA waste can be a highly beneficial approach for large-scale industrial implementation.

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Investigating Plasmonic Catalysis of C-C/C-N Coupling Reactions in Water using Bi-Metallic Ag-Cu/Ag-Co Substrates via In-Situ SERS

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Abstract

Solar energy-driven photochemical reactions can be catalysed by certain metal nanoparticles such as Au, Ag, Cu, which enhances light-matter interaction via localized surface plasmon resonances (LSPR). This is termed plasmonic catalysis.^{1,2} On decaying, the LSPRs can generate hot carriers, which are highly energetic species that trigger chemical transformations in the molecules embedded on the surface of the metal nanostructures. These chemical reactions can be expanded by coupling plasmonic metals and catalytically active metals. In this study, we alloy plasmonically active Ag with economic plasmonic metal copper (Cu) and catalytically efficient however non-plasmonic transition metals, such as cobalt, rhodium, and iridium (i.e. Ag-Cu, Ag-Co, Ag-Rh, and Ag-Ir) and use them in plasmonic catalysis. The phenomenon of LSPR also enhances the Raman signal of analyte molecules adsorbed on the substrate, ensuring that the catalytic study can be investigated using in-situ Surface Enhanced Raman Spectroscopy (SERS). The aforementioned bimetallic nanostructures are prepared by simple thermolysis of metal-alkyl ammonium halide precursors and are thoroughly characterized thereafter using various spectroscopic techniques, such as, UV-Vis spectroscopy, X-ray photoelectron spectroscopy (XPS), energy-dispersive X-ray fluorescence (ED-XRF), X-ray diffraction (XRD) and scanning electron microscopy (FESEM). The ED-XRF studies confirm the alloying for the bimetallic substrates. However, since there is an immiscibility gap in the phase diagram of the plasmonic metals with the non-plasmonic transition metals, the uniformity in the alloying cannot be confirmed which remains a challenge while preparing such bimetallic substrates. Regardless, owing to their excellent catalytic properties and unique SERS sensitivity of Ag, we demonstrate a facile approach to monitor and determine the reaction kinetics of C-C/C-N coupling reactions.³ Three different laser excitation sources: 457nm, 532nm and 632.8nm are used to inspect the reactions. Herein, we try to understand the role of plasmon-induced 'hot-carriers'⁴ in the formerly mentioned photo-reduction and photo-oxidation reactions using various scavenging solutions on our substrates. As these self-coupling reactions are very important class of reactions used in fine chemical and pharmaceutical industries but are mostly performed using conventional palladium-supported catalysts, it is necessary to find a more lucrative approach to perform and investigate the mechanism of such reactions.

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Plasmon-mediated Green Hydrogen from Organosilane Waste Under Sunlight with Value-Added Co-Products

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Abstract

An effective strategy for efficient and on-site production of green hydrogen from waste materials¹ and renewable energy resources could mitigate the cost associated with hydrogen transport and storage^{2,3}. In this study, we establish gold nanoparticle-enabled photocatalytic organosilane hydrolysis as an effective strategy for on-demand green hydrogen production from sunlight without need of any external bias or electricity. Besides green hydrogen production, we also report on photocatalytic synthesis of cyclosiloxanes and ladder-like polysilsesquioxanes as value-added by-products which also have extensive academic and industrial applications. We demonstrated that this photocatalytic system works with entire visible and NIR spectral range with maximum IPHCE reaching up to 0.66% at 808 nm. The strategy also shows great activity on panel of silanes, primary silane producing 2.8 times more hydrogen than a tertiary silane. Finally, the catalyst was subjected to a practical assessment under natural sunlight, where we achieved hydrogen production rate of 90 l/m²/day from active area of 48 cm². The robustness and easy scalability of the catalyst, no requirement of any external electricity source, and value-added by-products uniquely place our strategy for further development of an on-demand domestic-scale solar-powered hydrogen production system.

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Ir³⁺ or Ir⁴⁺: Intriguing Role of Ir Valence State on The Photocatalytic H₂ Generation in Visible-Light Absorbing Ir-Doped BaTiO₃

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Abstract

Scalable sunlight-driven H₂ production using photocatalyst modules has already been demonstrated.¹ However, the need of the hour is to design a next-generation photocatalyst to achieve >5% solar to hydrogen energy conversion efficiency. In this direction, understanding the factors governing the H₂ generation^{2,3} and designing visible-light absorbing photocatalysts are essential. Our recent work focused on elucidating the photocatalytic H₂ production in BaTiO₃ (BTO). Despite many advantages and prospects, BTO has a wide band gap capable of harnessing only UV light. Hence, BTO is doped with iridium (Ir) at Ti sites to extend the optical response towards the visible region. Detailed structural and optoelectronic analysis revealed the intriguing role of the Ir dopant's valence state on the photocatalytic H₂ evolution.^{4,5} Simply reducing the band gap of BTO via doping does not necessarily enhance the photocatalytic H₂ evolution. Results highlight the importance of the energetic position of the dopant within the band gap and its electron occupancy on the H₂ generation

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Efficient Photocatalytic CO₂ Reduction of the AsXBr (X= S, Se and Te) Heterostructures

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Abstract

This study introduces a novel approach for photocatalytic CO₂ reduction utilizing the recently predicted ternary chalcogenide halides, AsSBr, AsSeBr, and AsTeBr. These materials exhibit promising electronic properties, including direct band gaps of 1.56 eV, 1.47 eV, and 1.76 eV, respectively, making them ideal candidates for light-driven CO₂ conversion. To assess the stability and catalytic performance of these materials, we conducted first-principles calculations. Our results demonstrate that AsSBr, AsSeBr, and AsTeBr possess favorable thermodynamic stability, with cohesive energies of -2.53 eV, -2.40 eV, and -2.31 eV, respectively. Furthermore, phonon calculations confirm their structural stability. We investigated the interaction of these materials with CO₂ molecules and found that pristine AsSBr, AsSeBr, and AsTeBr exhibit weak binding affinity. However, the introduction of single-atom catalysts (SACs) significantly enhances CO₂ adsorption, suggesting their potential to improve the efficiency of the photocatalytic process. Our findings highlight the potential of AsSBr, AsSeBr, and AsTeBr as promising photocatalysts for CO₂ reduction. Further investigations into the design and optimization of SACs on these materials could lead to the development of highly efficient and selective catalysts for sustainable energy production.

Intriguing Role of N-Vacancies And p-States in Extending the Optical Absorption and Photocatalytic H₂ Evolution in Copolymerized G-C₃N₄

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Abstract

Due to its metal-free polymeric nature, ease of synthesis using low-cost precursors and tunable optoelectronic properties, graphitic carbon nitride (GCN) is extensively used as a photocatalyst to convert solar energy to chemicals and fuels. Despite these prospects, GCN demonstrates inefficient photocatalytic performance, partly attributed to its inadequate light absorption.¹ To address this challenge and to utilize the full potential of GCN, extending its absorption edge beyond 460 nm is crucial. In this direction, copolymerization is one of the approaches predicted to increase the degree of conjugation, thus redshifting the optical absorption.² In this work, GCN is copolymerized with different types of comonomers to extend the optical absorption to 550 nm. The copolymerized GCN demonstrated an enhanced photocatalytic H₂ evolution rate under 500 nm excitation, while pristine GCN was inactive. The formation of N-vacancies and/or π states upon copolymerization and their effect on the structural and optoelectronic properties was rationalized. Furthermore, a correlation between the mechanism of (co)polymerization, electronic nature of the defects formed, origin of extended absorption and photocatalytic H₂ evolution rate in copolymerized GCN was elucidated. Results offered rational insights into the factors limiting the performance of GCN which will aid in enhancing the H₂ generation efficiency further.

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Investigating the Effect of Various Process Parameters on Visible Light-Driven TiO₂-based Photocatalysis for the Remediation of Aqueous Phase Polystyrene Microplastics

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Abstract

The existence of microplastics (MPs) in marine and terrestrial environments is increasing tremendously. Due to their size (<5 mm), MPs could easily pass through the filtration processes of typical water treatment plants and ultimately reach surface water. On the other hand, due to their vast surface-to-volume ratio and chemical properties, MPs could adsorb hazardous substances from their adjacent environment. Further, these MPs, along with harmful contaminants, can enter the human body through lower trophic levels and threaten human health. Moreover, the methods generally used to separate macroplastic waste are unsuitable for MPs. Therefore, photocatalysis is considered as an alternative technique to treat MP pollution in an aquatic environment. Though the photocatalytic degradation of MPs has been reported, the effect of various process parameters on the photocatalytic degradation process has not been significantly investigated. To fill this research gap, the impact of different experimental parameters on the photocatalytic degradation process of polystyrene MPs was investigated using modified TiO₂, heterojunctioned with carbon nanotubes (CNT)) under visible light irradiation. Further, photodegraded samples were analyzed using a turbidity meter, FTIR, TOC analyzer, and GC-MS analysis to determine the effectiveness of the photocatalyst. A detailed qualitative and quantitative analysis of degradation studies of MPs will be presented at the conference.

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Fluorinated Transition Metal-Based MOF with Enhanced Water Stability for Efficient CO₂ Reduction

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Abstract

Rising atmospheric CO₂ levels have led to an imbalance in the natural carbon cycle.^{1,2} One of the best approaches to maintaining the anthropogenic carbon cycle is the catalytic conversion of CO₂ into certain useful chemicals. Due to their industrial demands, the conversion of CO₂ into CO and other liquid/gaseous products is of utmost importance. In the present work, we have strategically designed a fluorinated transition metal-based MOF with tuned chemical properties and exposed catalytic active sites for CO₂ conversion.³ The presence of amide moieties improved the material's electronic conductivity, whereas the fluorine groups enhanced the MOF's moisture stability. The judicious tuning of the catalytic features via incorporating functional groups significantly improved the MOF's catalytic performance for CO₂ reduction.^{4,5} Detailed structural characterization of the MOF and catalytic experiments were performed thoroughly to reduce CO₂ into the desired product.

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Diphenylanthracene-based Trimeric Systems for Efficient Photon Upconversion through Triplet-Triplet Annihilation

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Abstract

Materials that can transform the lower energy photons into higher energy ones find applications in a broad range of light driven devices/processes. They can be used to improve the efficiency of solar cells, or be applied in bioimaging or light-triggered drug release etc. Among the various available methods to perform photochemical photon up conversion, the triplet-triplet annihilation-based photon up conversion (TTA-UC) offers a unique advantage over other methods such as two-/multi-photon absorption (TPA) or second harmonic generation (SHG) which is the capability of upconverting incoherent light. Unlike SHG or TPA where extremely high energy source ($\sim \text{GW}/\text{cm}^2$) is required, TTA-UC can successfully upconvert the lower power radiation ($\sim \text{mW}/\text{cm}^2$). For any upconverting system, it is desirable to have high upconversion quantum yield (Φ) and a low threshold intensity (I_{th}).

As TTA-UC depends upon triplet fusion, which is usually diffusion-controlled process, it becomes extremely challenging to get good and I_{th} values at dilute conditions. An intramolecular triplet fusion (iTTA) may help in improving the efficiency of upconverting system significantly. We have prepared three trimeric molecular systems based on 9-Phenylanthracene and 9,10-diphenylanthracene units and showed that in such systems up conversion can be achieved through a contribution from inter- and intra-molecular triplet fusions simultaneously.

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Construction of Imine-linked Nanoparticle Organic Networks for Field Effect Transistors

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Abstract

Metal nanoparticles (MNPs) have revolutionized material science on account of their impressive extent of applications. But MNPs often exist as homogeneous fine colloidal dispersions, which limits their applicability in heterogeneous catalysis, electronics, sensing, etc.¹ Various strategies with varying degrees of success have been adopted over the years for the heterogenization of MNPs, including anchoring and/or encapsulation of MNPs in polymers, zeolites, silica, etc. However, these strategies suffer from unavoidable drawbacks like leaching and agglomeration-induced deactivation. In this work², we have introduced a reticular chemistry approach to heterogenize MNPs as networks [nanoparticle organic networks (NONs)] by reacting amine-functionalized MNPs (as nodes) with dialdehydic linkers (as organic struts) via a green, sustainable, and facile mechanochemical Schiff base condensation.³ The possibility of structural modulation with a variety of MNPs and a diverse array of covalent linkages would make this approach highly promising. In addition, capitalizing on the excellent optoelectronics of MNPs, NON-semiconducting polymer (SP) composite material-based field effect transistors (FETs) were fabricated. The results showed an enhancement of the in-plane charge transport mobility and a stupendous increase in photoresponsivity upon incorporating NONs into the semiconducting polymer matrix.

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Sr-doped MoO₃ for Photocatalytic N₂ Fixation

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Abstract

Ammonia, an integral part of sustainability, has drawn huge attention, being the most essential chemical fertilizer, a component for industrial chemicals, and a zero-carbon fuel. Ammonia production by the conventional Haber–Bosch process requires high temperature and pressure leading to immense energy consumption and environmental issues. In this context, photocatalytic N₂ fixation utilising solar energy and N₂ and H₂O as raw materials has evolved as a promising, ecofriendly, and cost-effective strategy. To drive the N₂ reduction, enough affinity for chemisorption and molecular N₂ activation is required which can be achieved by using an ideal photocatalyst.¹ Amongst, metal oxides have ignited enormous attention and creating defects by heteroatom doping can enhance light absorption and provide multiple active sites.^{2,3} In this aspect, we have developed a Sr-doped MoO₃ photocatalyst to produce NH₃ from pure water. A detailed analysis of the as-synthesized photocatalyst has been conducted using various characterization techniques, confirming their structural, optical, electrochemical properties, and their promising activity for the photocatalytic N₂ fixation reaction. Furthermore, multiple control reactions were conducted to better understand the process and a suitable mechanism for the reaction has been proposed. The work paves the foundation for selective photocatalytic nitrogen fixation and paramount production of NH₃.

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Thermally Stable Li⁺ co-doped ZnMoO₄: Eu³⁺ Phosphors for White LED Applications and Selective Sensing of Nitroaromatic Compounds

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Abstract

A series of Zn_{1-x}Eu_xMoO₄ (0.01 ≤ x ≤ 0.11) and Zn_{0.91-x}Li_xEu_{0.9}MoO₄ (0.01 ≤ x ≤ 0.05) phosphors was synthesized. The PL intensity of the Zn_{1-x}Eu_xMoO₄ phosphors increases on increasing Eu³⁺ concentration and then gradually decreases after 9 mol% of Eu³⁺ concentration because of quenching through electric multipolar interaction.

The emission intensity was further enhanced by co-doping with the monovalent Li⁺ ion due to the local distortion of the crystal field surrounding the Eu³⁺ activator. Furthermore, color purity and quantum yield for 3 mol% Li⁺ co-doped sample is found to be 92 % and 79 %, respectively. This shows that the phosphors are potential materials for red lasers and White LEDs applications.

It was observed that the Zn_{0.88}Li_{0.03}Eu_{0.9}MoO₄ phosphor has high thermal stability, i.e., 68 % @ 300 °C. In this work, a facile fluorescence method was developed to detect para-Nitrophenol (p-NP), a toxic pollutant. A linear response was obtained over the concentration range from 1 nM to 200 μM with a low detection limit of 12 nM for para-Nitrophenol. The inner filter effect (IFE) was found to be the mechanism for sensing. More importantly, this method has the potential to detect p-NP assay in real water samples.

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Halide-Dependent Regulation of Energy and Electron Transfer in CuInS_2 -Decorated Perovskite Nano-heterostructure

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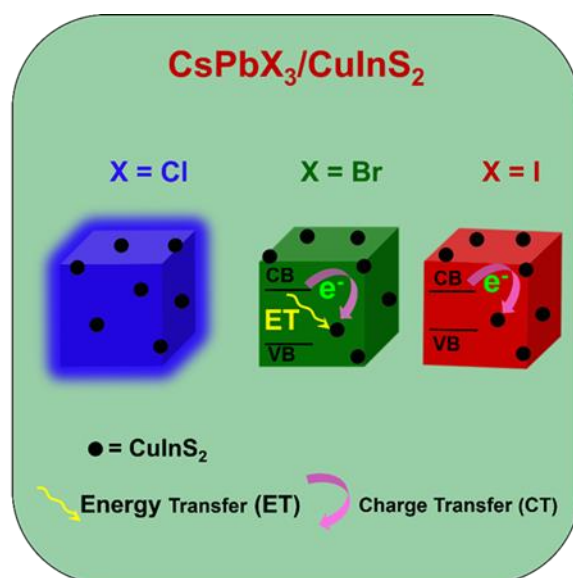
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Abstract

Nanoheterostructures based on perovskite nanocrystals (NCs) are emerging as strong contenders in semiconductor research. This study presents the fabrication of a type II $\text{CsPbX}_3/\text{CuInS}_2$ ($\text{X} = \text{Cl}, \text{Br}, \text{or I}$) perovskite/multinary chalcogenide quantum dots (QD) nanoarchitecture to investigate the energy and charge transfer (ET and CT, respectively) processes.¹ Optical measurements of $\text{CsPbX}_3/\text{CuInS}_2$ (CPX/CIS) revealed efficient photoluminescence (PL) quenching of the parent CsPbX_3 for $\text{X} = \text{Br}$ or I , with a two-order lower PL quenching for $\text{X} = \text{Cl}$. Spectral overlap and thermodynamic band alignment analysis suggest the PL quenching mainly results from the ET process from CPBr NCs to CIS QDs while exclusively interfacial CT process from CPI NC to CIS QDs is active. Contrary to the driving force ($-\Delta G$) for the CT process, the $\text{X} = \text{Cl}$ system exhibits a reverse electron transfer order, for which we propose the CT occurs in the Marcus inverted region. This halide-dependent controlled regulation of CT and ET processes in these nano heterostructures holds potential for advanced optoelectronic applications.



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Structural and Theoretical Investigation of Photophysical Properties in Anthracene-Cyanostilbene Based Donor-Acceptor Systems

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Abstract

Cyanostilbene systems obtained paramount interest among various π -conjugated systems owing to their fascinating fluorescence properties in the solid state.¹ The cyanostilbenes attached with various functional groups were explored for their aggregation induced emission (AIE) and multistimuli responsive nature.² Herein, we report the synthesis and photophysical properties of highly emissive donor-acceptor systems based on anthracene and cyanostilbene, carrying hexyl (**CSB-1**) and dodecyl (**CSB-2**) chains. The molecules are highly emissive in both solid and solution states owing to intramolecular charge transfer and AIE respectively. The molecule **CSB-1** showed stress induced emission switching and solvent induced recovery attributed to the change in crystallinity under applied stimuli. The observed photophysical properties of **CSB-1** is compared with that of **CSB-2** and substantiated with the structural and packing details obtained from single crystal X-ray diffraction and DFT calculations.³ The higher quantum yield shown by **CSB-1** in the solution state is substantiated by further theoretical studies explaining the tailored photophysical characteristics through a comprehensive understanding of the intricate structural dynamics at the minimum energy conical intersection (MECI) points and their significant influence on fluorescence properties. The results revealed that the relative positioning of conical intersections, where the electronic ground and excited states intersect in the potential energy space, determines the non-radiative decay process in this compound.⁴ Thus, this study offers valuable insights into the factors that contribute to the quantum yield of this organic π -conjugated material and the molecular design of photofunctional devices based on such materials.

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Construction of Inverse Vulcanized Sulfur Polymer embellished with Silver Nanoparticles for SERS Screening of Hazardous Colorants and Antibiotic in Contaminated Water

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Abstract

Surface-enhanced Raman spectroscopy (SERS) has become a hot topic in the research field which gaining more attention day by day. It is important to design a smart SERS substrate in order to implement the SERS technology in real-world applications. This study introduces a chemically and thermally stable polymer nanocomposite in which waste sulfur, functionalized with vinylic monomer (1,3- diisopropenylbenzene (1,3-DIB)) via inverse vulcanization^{1,2}, is integrated with silver nanoparticles (Ag NPs). The sulfur-enriched nanocomposite effectively stabilizes Ag NPs, providing additional hotspots that enhance the efficiency of the SERS substrate. The average particle size of distributed Ag NPs on polymer surface was found to be 22.16 nm. This developed SERS platform exhibited exceptional SERS signal enhancement for detecting two organic dyes, methyl red (MR) and methylene blue (MB), with ultralow detection limits of 0.06 μM and 2.14 μM , respectively. Additionally, it successfully determined the antibiotic, ciprofloxacin (CIP) as low as 0.79 μM . Experimental findings revealed the relative standard deviation (RSD) of S/DIB/Ag substrate was 4.55%, showing its excellent spot to spot uniformity. The proposed SERS sensor involved easy, low-cost fabrication process and showcased high stability, reproducibility, and detection efficiency suitable for diverse analytical applications.

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Spectroscopic Evidence of Improper H-Bonds Formed in Alkanolamines Used in CO₂ Capture

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Abstract

The growing levels of CO₂ in the atmosphere have been a matter of great concern since CO₂ is considered as a potential greenhouse gas. In an effort to lower the rising levels of CO₂ in the atmosphere, techniques like carbon capture were introduced. Carbon capture and utilization (CCU) not only helps in storing CO₂, but also utilizes the stored CO₂ to produce value added chemicals. Aqueous alkanolamines have been widely used on a commercial scale as CO₂ absorbents. In this work, we report a detailed Raman spectroscopic study of a primary alkanolamine used in carbon capture and highlight the changes taking place at the molecular level in the presence of water and CO₂. A prominent blue shift in the C-H stretching regions in the presence of water is observed which can be explained on the basis of the formation of improper hydrogen bonds between water and the C-H groups of the alkanolamine. After reaction with CO₂, formation of a carbamate further results in blue shifts, observed keenly in the C-H stretching region due to a synergistic effect of hydrogen bonding and the mesomeric effect of the carbamate group. Through our study, we provide herein a detailed spectroscopic analysis of changes occurring in alkanolamines before and after carbon capture.

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Influence of Dimensionality on Optical Properties of Doped Assembly of Gold Nanoclusters

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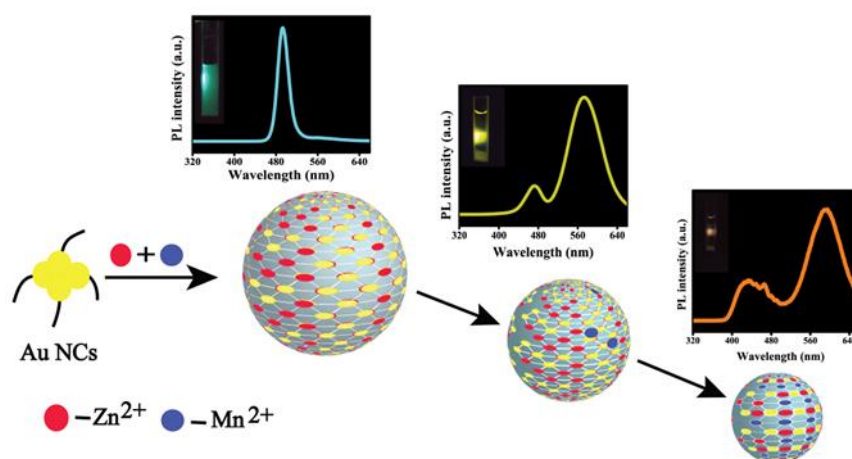
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Abstract

In this work, we successfully doped Mn^{2+} ions into zinc-mediated assemblies of gold nanoclusters (Zn Au NCs), leading to the emergence of luminescence from the dopant Mn^{2+} ions. This was accompanied by the simultaneous quenching of the original luminescence of the Zn Au NCs. The chemical doping of the Zn Au NCs assembly with Mn^{2+} ions took place progressively during the synthesis process with concomitant changes in the size of the assembly, which resulted in sequential changes in the optical properties of the Mn^{2+} doped Zn Au NCs assembly. Careful monitoring of changes in optical properties during the synthesis provided valuable insight into the doping process. In addition, due to the presence of Mn^{2+} ions, the doped Zn Au NCs assembly exhibits size-dependent superparamagnetic behavior in addition to optical properties, making it a promising magneto-optical material.



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High-Pressure SERS Effect on ZIF-67/R6G System

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Abstract

High-pressure (HP) effects on surface-enhanced Raman spectroscopy (SERS) is a new-prospect due to the importance of pressure as an external stimulus that can tune the lattice and electronic band structure of the SERS substrate and analyte molecule. Here, we have used ZIF-67 as the PI-SERS substrate and selected rhodamine R6G molecules as analyte to explore the analyte Raman signal enhancement in both compression and decompression cycles. SERS results demonstrate an enhancement in the SERS signal intensity with an increase in pressure and show maxima at 0.12, 0.38 and 1.12 GPa. The initial enhancement at 0.12 GPa is interpreted as mainly due to molecular resonance through pressure-induced blue shift of the photoluminescence (PL) wavelength of R6G. HP synchrotron XRD study on the ZIF-67/R6G system illustrated an initial expansion of the ZIF-67-unit cell due to the inclusion of R6G molecules inside the pores and a structural phase transition around 0.38 GPa followed by an irreversible amorphization around 3 GPa. The pressure release from a maximum pressure of 6.42 GPa, is observed to provide a significant SERS enhancement. Although the crystal lattice seems to collapse irreversibly with HP, Raman studies indicate the recovery of the phonon modes upon pressure release.

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Synthesis of Kraft Lignin-Based Conductive Resin and its Application in Sensor and Flexible Electronics

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Abstract

Lignin, an aromatic component of lignocellulosic biomass, is known as cheap, renewable, and environmentally beneficial. Lignin is the second-most natural polymer after cellulose on earth, it has a high carbon content. The industry produces around 50 million tonnes of lignin each year. These characteristics include chemical reactivity, UV shielding, antibacterial, biodegradability, and anti-oxidation. Finally, considering the unique properties of lignin and the need for high-quality flexible electronics, some recommendations are provided for future research and development areas in lignin-based conductive resin electronic devices. First, we extract the lignin from the black liquor, modify the lignin, and synthesize lignin-based conductive resin. To characterize lignin and lignin-based conductive resin. Increasing sulfur content in lignin improves synthesis and leads to a modest improvement in conductivity. Furthermore, I employed CNT to improve conductivity at the desired peak. Our investigation of Kraft lignin and conductive resin, including FTIR, TGA, DSC, GPC, DLS, FESEM, EDX, zeta potential, showed their good electrical conductivity Overall, conductive resin has numerous benefits, including flexibility, printability, customization, low cost, integration, sustainability, versatility, and durability, making it a popular choice for electronic devices manufacturing and inventive product creation. The application of lignin-based conductive resin in environment sensor, flexible electronics, flexible packaging, electronic packaging, and anti-counterfeiting for pharmaceutical packaging.

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pH Dependent Study of Isatin Based Drugs using Raman Spectroscopy and SERS

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Abstract

The molecular structure of Isatin drug and its derivatives such as 1-Misa, 1Phisa, 5-Fisa, and 5-Iisa molecules have orange or reddish color in solid or liquid state but the change in color was observed after the addition of alkaline pH. Raman study of Isatin and its derivative shows the structural change in basic medium at different laser source (532, 633, and 785 nm), and this change was also observed by UV-visible spectroscopy. The characteristic features of Isatin and its derivatives due to the effect of pH demonstrate that these drugs can losses their original properties through the transformation of Isatin into anthranilic acid. Moreover in this work, we have synthesized bismuth oxide nanoparticles via hydrothermal method¹ and used as a SERS substrate for the quantitative analysis of the considered drug molecules. The SERS activity of α -Bi₂O₃ substrate was performed by the detection of Isatin with the lowest detection limit at 100 μ M shows good results like Ag NPs² with 1mM. Further the DFT calculation was applied to assign the vibrational modes of the experimental Raman spectra.

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Coherent Phonons and Charge Carrier Localization in Cesium Gold Bromide

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Abstract

Halide perovskites (HPs) are promising materials for opto-electronic applications due to their unique electronic and vibrational properties. Electron-phonon coupling in conventional lead-based HPs leads to interesting photo-induced non-equilibrium dynamics, such as the slowing down of electronic relaxation by equilibrium with hot phonons.¹ However, the toxicity of lead-based HPs necessitates the exploration of lead-free alternatives. This study investigates photo-induced processes in caesium gold bromide films using femtosecond transient absorption (TA) and Raman spectroscopy. We elucidate inter-valence charge transfer states² and their coupling to the lattice, explaining the pronounced oscillations in the TA signal lasting several picoseconds. Raman spectroscopy identifies optical and acoustic phonon modes of the crystal that are excited, leading to coherent phonon modulation of the TA signal. We explain the coupled dynamics of electronic states and coherent phonons during the early stages, leading to the formation of a localized polaronic state over tens of picoseconds. The strong electron-phonon coupling and slow dephasing of coherent phonons point towards slow vibrational relaxation and suggest a lower rate of heat dissipation,³ making this material a promising testbed for studying optical control of electronic and lattice dynamics

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Probing the Fluorescence Intermittency of Bimetallic Nanoclusters using Single-Molecule Fluorescence Spectroscopy

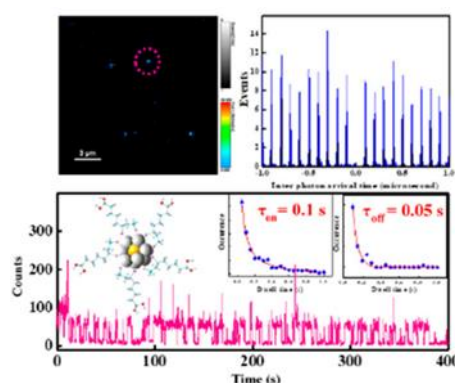
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Abstract

Single-molecule spectroscopy (SMS) is a unique and competent technique to study molecule dynamics and sense biomolecules precisely. The design of an ultrahigh-stability single fluorophore probe with excellent photostability and long-lived dark transient states for single-molecule fluorescence microscopy is challenging. We found that the photostability of bimetallic AuAg₂₈ nanoclusters is better than monometallic Ag₂₉ nanoclusters. The photon antibunching experiments unveiled exceptional brightness and remarkable photostability with high survival times of up to 218 s with minimal blinking. AuAg₂₈ NCs exhibited longer “on” times and shorter “off” times as compared to Ag₂₉ NCs. The statistical analysis was performed on at least 100 molecules that showed single-step photobleaching and almost a 5-fold enhancement in intensity on Au doping in Ag₂₉ NCs. The distinctive and tunable photophysics of metal NCs can offer huge potential in pushing single-molecule dynamic measurements to be carried out biologically.



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Triboelectric Nanogenerators Enhanced by a Metal-Organic Framework for Sustainable Power Generation and Air Mouse Technology

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Abstract

Enhancing the output performance of triboelectric nanogenerators (TENGs) can be effectively achieved by designing materials as active fillers into the polymer with high triboelectric properties. Recently, exploration of metal-organic framework (MOF) based TENGs has attracted attention due to their triboelectrification properties and charge trapping ability. Here in this work, we have synthesized a Cd-MOF, which acts as a filler, prepared by employing 2-aminoterephthalic acid (2-ATA) and conjugated nitrogen-containing 4,4'-azopyridine (AzPy) ligands which help to improve the output performance of the TENG device. The new Cd-MOF was characterized by microscopic analysis and authenticated by single-crystal X-ray diffraction (SC-XRD) studies. Furthermore, the MOF was incorporated with polydimethylsiloxane (PDMS) to construct MOF/PDMS film and utilized for the TENG study. The trapping ability was analyzed through KPFM studies. The MOF-TENG generated a maximum output power density of 0.124 W m^{-2} . The MOF-TENG device was attached to the fingers of a glove and used to control the mouse movement in a computer *via* finger movements. This strategy provides a new avenue for the preparation of new-generation fillers for more active electrification and trapping.

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Aggregation and Crystallization Studies of DNA Functionalized Nanoparticle for Enhanced Optical Response

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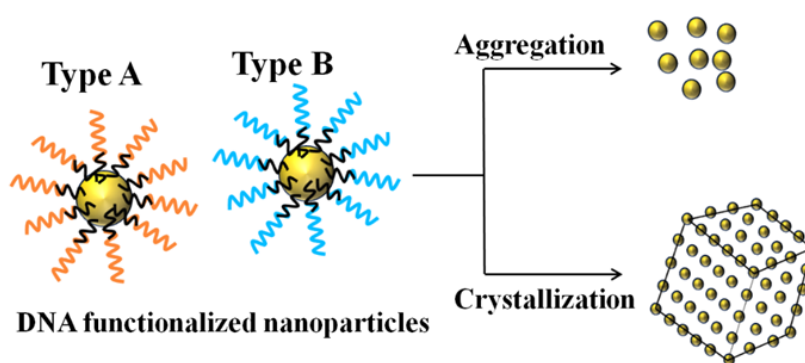
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Abstract

Our study delves into the comprehensive investigation of DNA-functionalized nanoparticles colloids focusing on variations induced by different DNA chain lengths and different sizes of nanoparticles. The study examines these particles both in their colloidal aggregates and crystallized forms providing crucial insights into their aggregation behavior and stability. By functionalizing nanoparticles of varying sizes with different DNA chain lengths, we explore their interaction dynamics using techniques such as dynamic light scattering, UV-visible spectroscopy, and optical microscopy. These methods help not only to observe the aggregation patterns but also to optimize the parameters for effective crystallization of the DNA-nanoparticle assemblies. The optimized crystals are then analyzed using optical microscopy and small-angle X-ray scattering to uncover their crystallographic properties, with electron microscopy offering a deeper look at their internal arrangement. Finally we demonstrate that the structural quality of DNA-nanoparticle crystals directly influences their surface-enhanced Raman spectroscopy (SERS) activity. This correlation suggests that these crystals have great potential for applications in analytical chemistry and biosensing. Our findings offer a deeper understanding of the growth mechanisms and properties of DNA-AuNP crystals, laying the groundwork for their development as innovative optical materials and high-performance sensing platforms.



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Room-Temperature Polaron Dynamics in Lead-free $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ Layered Double Perovskite Nanocrystals

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Abstract

In search of lead-free halide perovskites, a novel class of perovskites known as double-perovskites, has emerged. In this work, we investigate the effect of surface capping ligand oleylamine on the excited state dynamics of $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ CCSC [1] nanocrystals (NCs) using femtosecond transient absorption spectroscopy (fs-TAS), along with computational studies. Furthermore, the coupling of charge carriers to coherent low-frequency phonon modes, which influence relaxation dynamics and thereby control photovoltaic performance, is studied using broadband time-resolved impulsive-stimulated Raman spectroscopy (broadband TR-ISRS). In ISRS, excitation by an ultrashort Raman pump pulse (620 nm) induces coherent phonons via Raman scattering. Subsequent probe-light interaction produces a time-dependent modulation of transmission, and Fourier transform of the signal provides a vibrational Raman spectrum [2-3]. Further, an actinic pump pulse (centered on 400 nm) is introduced to obtain a series of Raman spectra by varying the time delay between the actinic and the Raman pump pulses. It primarily displays two modes: one from CCSC NCs at 283 cm^{-1} and another mode originating from the solvent (hexane) at $1,040\text{ cm}^{-1}$. It is shown that the relative intensity variations of the NC mode compared to the solvent mode. The time component obtained from fitting the data aligns well with the time scale from the global analysis of fs-TAS data, indicating a phonon-mediated decay of photo-generated hot charge carriers.

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Forcing Isomerization Pathways to Completion inside Water-soluble Nanocages

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Abstract

Cis-trans photoisomerization is a basic photochemical reaction that is vital to the functioning of many biological processes, including light sensing, ion pumping and vision.¹ Thus far, photoisomerization has been exploited in backbones of molecular switches to activate many artificial light-energy conversion systems and regulate in-vivo biochemical pathways. The secret is in the reaction timescales which are usually ultrafast affecting substantial global conformational change. Although isomerization has been used in diverse applications, one fundamental bottleneck is producing 100% yield of one of the isomer after light-activation for any photoswitch. The problem lies in overlap of the absorption spectra of cis-trans forms of the photoswitch.² To solve this major challenge, we have developed a new method to control the outcome of cis to trans isomerisation in stilbene derivatives using visible light and water with high efficiency inside confinement. Furthermore, with the help of time resolved spectroscopy, we have tracked the reaction pathway and assigned the intermediates formed to be radical cations of cis and trans stilbene molecules.³

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Photocatalytic H₂O₂ Production by Heptazine Hydrazine Polymer

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Abstract

Hydrogen peroxide (H₂O₂) plays a crucial role in various applications, and it can be used as clean energy source.¹ Currently, H₂O₂ is primarily manufactured using the indirect anthraquinone method, known for its significant energy consumption and the generation of by-products. The photocatalytic synthesis of H₂O₂ enabled greener, on site and on demand H₂O₂ production under mild conditions. Carbon nitride (CN) is known to produce H₂O₂ with very high selectivity.² But its narrow light absorption and fast charge recombination shadow its photocatalytic potential. To overcome these demerits of CN and increase the efficiency of H₂O₂ production, we synthesize a heptazine based covalent organic polymer (COP). It enhances light absorption and charge separation. In my poster I will discuss the attempts we made to synthesis a heptazine COP by mechanochemical methods for photocatalytic H₂O₂ production. Using chemical methods along with various spectroscopic tools like EPR, photoluminescence and transient absorption studies we have tried to reveal the mechanism pathway of this photocatalysis.

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Mid-Infrared Active Non Toxic Colloidal Quantum Dots

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Abstract

Infrared technology has found widespread applications across various fields, where conventional semiconductor alloys like InGaAs, $\text{Hg}_x\text{Cd}_{1-x}\text{Te}$, and InSb have been widely utilized as active materials in devices. However, the manufacturing and assembly processes for these materials are intricate and costly. To address these challenges and potentially replace expensive epitaxially fabricated devices, colloidal quantum dots (CQDs) have emerged as promising alternative. We developed non-toxic n- Ag_xSe ($x>2$) CQDs exhibiting intraband transition (1S_e - 1P_e) in mid-infrared regime. We believe that shedding insights on the intraband relaxation pathways is of paramount importance for further design and optimization of the materials and the devices thereof. We sought therefore to investigate the intraband carrier dynamics of n- Ag_xSe CQD, using a state-of-the-art mid-infrared fs-transient absorption spectrophotometer. We evaluated the intraband exciton life-time and multicarrier interaction in both solution and thin film states of three different Ag_xSe in sub-ps timescale. This investigation is poised to advance the fundamental study of intraband excitons in ultrafast time scale as well as infrared device community to enhance the performance of Ag_2Se -based devices by incorporating required modifications in near future.

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Triplet Harvesting TADF Emitters Towards Energy-Efficient Organic Electronics

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Abstract

Delving into precise exciton management in the subtle chemical design using organic materials and understanding key insights into organic electronics are of prime importance. The pioneering concept of thermally activated delayed fluorescence (TADF) could resolve the everlasting dilemma of spin statistics in achieving superior quantum efficiency of organic light-emitting diodes (OLEDs). Herein, we envisioned a simple design strategy combining short-range (SR) charge transfer (CT) with the main long-range (LR) CT excitation and synchronizing their complementary advantages to afford a new paradigm of hybrid multiple-resonant (MR) CT-type TADF emitters. D-A and D-A-D type emitters are constructed by modifying the auxiliary connection between the conventional carbazole donor and the oxygen-bridged tri-aryl boron-based acceptor core. These MRCT emitters are awarded superior photophysical properties including strong TADF emission in solution and thin films. The preferential horizontal orientation of the D-A-D structure significantly enhances out-coupling efficiency. Owing to their intrinsic merits, sky-blue electroluminescence with a record-high external quantum efficiency (EQE) is apprehended from a state-of-the-art OLED structure.

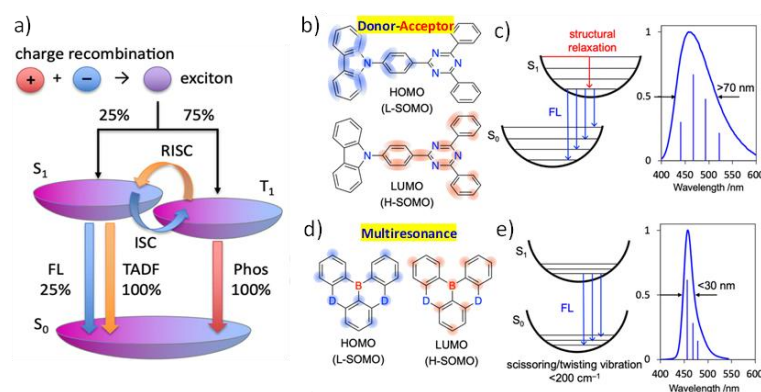


Fig. 1. (a) Schematic presentation of TADF mechanism. (b) Typical vibronic spectra for (b, c) D-A TADF and (d, e) MR-TADF emitters.

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Designing Electronically Tuned Defect-Rich Trimetallic-Ceria Catalytic Sites for Enhanced CO₂ Reduction Reaction

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Abstract

We developed a Ni-Cu-Zn/CeO₂ catalyst featuring a unique electron density distribution, achieved through the strategic integration of defects¹⁻³ and strong metal-support interactions (SMSI).^{2,3} This catalyst demonstrated exceptional performance, achieving a CO productivity of 49,279 mmol g⁻¹ h⁻¹ (equivalent to 10,484,894 mmol gmetal⁻¹ h⁻¹) at 650 °C—a nine-fold improvement over the best-reported catalysts. It also delivered outstanding CO selectivity of up to 99% and remarkable stability, with activity remaining unchanged even after 100 hours on stream at 500 °C. Furthermore, the reaction could be conducted effectively at temperatures as low as 350 °C. This raises an intriguing question: with conventional ceria and typical metal sites⁴⁻⁶, what makes this combination of trimetallic Ni-Cu-Zn sites and defective ceria support so exceptional? Insights from in-situ TEM and HERFD-XANES studies revealed the dynamic interactions and the distinctive electron density distribution between the CeO₂ support, its defects, and the trimetallic nanoparticles. The catalyst's extraordinary activity and stability arise from the synergistic interplay among the Ni-Cu-Zn sites and their SMSI with the defected ceria support. HERFD-XAS confirmed robust interactions between the trimetallic sites and the CeO₂ surface, a finding further supported by in-situ EELS data. These studies highlighted the critical role of ceria oxygen vacancies in both CO₂ activation and coke suppression during catalysis.

Real-time in-situ TEM imaging under catalytic conditions captured the movement and growth of active trimetallic sites, showing that their diffusion and sintering ceased once SMSI was established, even at elevated temperatures. These insights provide a groundbreaking perspective on catalyst design, emphasizing the transformative potential of defect engineering and SMSI in achieving unparalleled catalytic performance.

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Single Atom Induced Ferromagnetism for Magneto-electrocatalytic Water Splitting Reaction

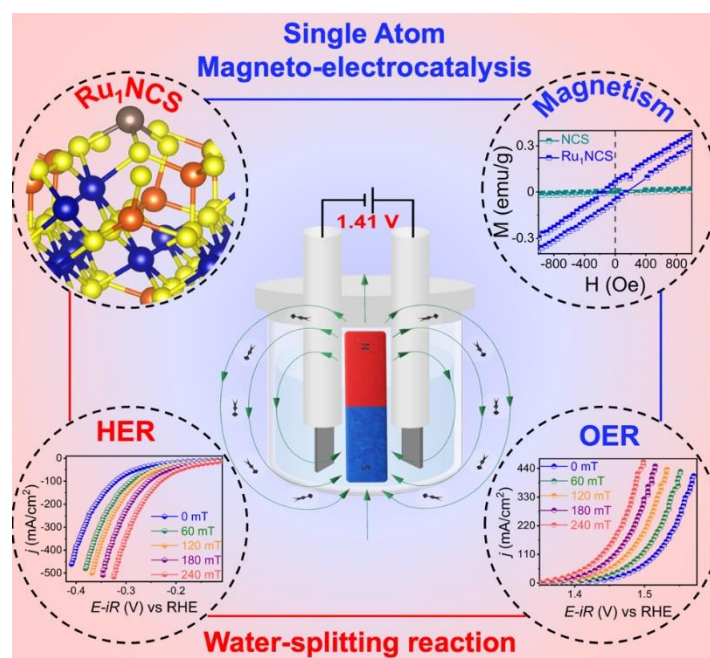
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Abstract

Single atom catalysts (SACs) have shown immense potential in green hydrogen production by effectively modulating the electronic properties of heterogeneous supports.¹ In this work, we have designed a Ruthenium single atom catalyst (Ru_1NCS) by taking Nickel-Cobalt sulfide (NCS) as active support material to improve the overall water splitting tendency via electronic as well as magnetic influence. The stabilization of atomic Ru has not only enriched the electronic property but also induced significant ferromagnetism to enhance the HER and OER activity by magnetohydrodynamic effect and spin parity conservation effect respectively. As a result of such para-to-ferro transformation, 32 mV and 36 mV reduction in overpotential has been observed for HER and OER activity respectively by applying just 240 mT of magnetic field. Moreover, a 12 % enhancement in the overall current density has also reduced the cell potential from 1.45 V to 1.41 V. A detailed study with time-dependent magneto-electrocatalysis has further scrutinized the real-time effect of magnetic field on overall catalytic performance. Simultaneously, the origin of magnetism and overall reaction mechanism has been successfully validated via density functional theory (DFT) and in-situ Raman studies.



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Ultrathin-Highly Twisted PdNi Alloyed Nanowires for High-Performance Fuel Cell Reactions

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Abstract

Achieving high electrocatalytic performance with significant stability using nanostructures is a daunting challenge, but is a necessity for the development of sustainable devices. In this work, we have designed ultrathin twisty Palladium nanowires, doped with Nickel (PdNi TNWs), for high-performance fuel cell reactions: cathodic oxygen reduction reaction (ORR) and anodic methanol oxidation reaction (MOR). The presence of Nickel tunes the *d-band* center of palladium for favorable binding of the reaction intermediates¹ and provides resilience from the poisoning CO adsorbates² generated during the MOR. The nanowire morphology imparts multiple contact points between the catalyst and the electrode surface, preventing its detachment, or agglomeration, resulting in superior stability³. The PdNi TNWs exhibited a MOR mass activity about 2 and 8 times higher than that of Pure Pd (Pd TNWs) and commercial Pt/C, respectively, and durability for 50 hours, with more than 60% retention in the current. Similarly, for the ORR, the PdNi TNWs exhibit an $E_{1/2}$ of 0.95 V vs. RHE, maintained over 200,000 catalytic cycles. The significance of the design strategy of 1D nanostructures with oxophilic Ni was further demonstrated by the varied-temperature electrochemical studies for investigating adsorption vs. desorption kinetics of various reaction intermediates involved in the reaction.

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Development of Manganese-Nitrogen-Carbon Bifunctional Electrocatalyst for Low-temperature PEM Fuel cell

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Abstract

Proton exchange membrane(PEM) fuel cells offer a clean and efficient energy solution, but their commercialization is hampered by the high cost of platinum-based catalysts. In this study, we synthesized green, facile, highly porous Mn-doped Nitrogen-Carbon(N-C) electrocatalyst as a viable alternative. The catalyst's unique manganese-nitrogen-carbon coordination structure not only delivers exceptional bifunctional activity for oxygen reduction and evolution reactions (ORR and OER) but also mitigates potential Fenton reactions. Our synthesized catalyst shows comparable performance with commercial Pt/C and RuO₂/C benchmarks, exhibiting a four-electron pathway for ORR and a Tafel slope of 19.8 mV/dec for OER with a comparable onset potential. Moreover, its high porosity, attributed large BET surface area and ample electrochemical active surface area, contributes significantly to its catalytic activity. The presence of a mixed oxidation state of Mn and high defects in the carbon matrix enhance the overall performance of the bifunctional electrocatalyst. These findings underscore the potential of Mn-doped N-C as a cost-effective and durable electrocatalyst for advancing PEM fuel cell technology. By employing a simple and scalable synthesis method, we have developed a green and efficient electrocatalyst that showcases the potential of non-precious metal catalysts in realizing low-cost fuel cell systems

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Sustainable Electrocatalytic Conversion of (M)ethanol to Sodium Carbonate: Leveraging Inexpensive 3d Metal Molecular Electrocatalysts

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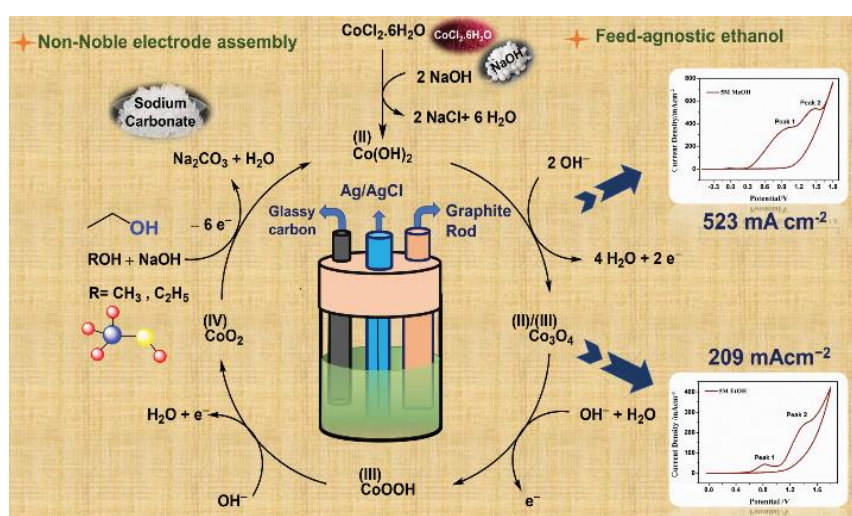
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Abstract

This study proposes a promising avenue for sustainable energy production through electrocatalytic oxidation of (m)ethanol using inexpensive homogeneous catalytic systems based on Ni/Co/Cr for use in direct alcohol fuel cells (DAFCs). Employing NaOH as the supporting electrolyte, we investigated metal salts and their bis(iminopyridine) complexes as anodic electrocatalysts for electro-oxidation of methanol and ethanol. Among these, $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ (10 mM) in a solution containing NaOH (6 M) emerged as the optimal electrocatalyst for both methanol and ethanol oxidation yielding current densities of $522.5 \pm 13.5 \text{ mAcm}^{-2}$ at 1.4 V Vs Ag/AgCl for methanol [5M] electro-oxidation and $209 \pm 25 \text{ mAcm}^{-2}$ at 1.34 V Vs Ag/AgCl for ethanol [5M] electro-oxidation. The electro-oxidation yielded carbon dioxide as the final product for both the alcohols, which was efficiently captured as sodium carbonate with an impressive yield of up to 97%, presenting a dual benefit of energy generation and greenhouse gas mitigation. This innovative system represents a significant leap forward in the design of sustainable, high-performance DAFCs. It not only demonstrates the potential for using earth-abundant metals in energy production but also offers a path to reducing environmental impact through the generation of valuable sodium carbonate, paving the way for a cleaner and more sustainable future.

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Effect of PCBM nanoparticles in Lead-based Layered (PEA)₂PbI₄ Perovskite Thin Films

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Abstract

Among different classes of halide perovskite materials, two-dimensional (2D) layered perovskites are considered one of the future potential semiconductor materials due to their higher moisture stability. However, the optical and electrical properties of the materials are still to be improved. The technique of additive engineering gives a scope to enhance the optoelectrical properties of the 2D perovskites. In this work, we study the impact of mixing a certain amount of a fullerene derivative '[6,6]-Phenyl C₆₁-Butyric acid Methyl ester' (PCBM) into 2D (PEA)₂PbI₄ perovskite thin films (PEA=Phenyl Ethyl Ammonium). The analysis shows that PCBM does not affect the structure and bandgap of the (PEA)₂PbI₄ perovskite. On the other hand, PCBM improves photoluminescence emission intensity and promotes charge separation at the perovskite/PCBM interface. Hence, PCBM plays a dual role when mixed with (PEA)₂PbI₄ perovskite: 1) as a defect healing agent and 2) as an electron acceptor. However, over continuous illumination under high intensity on the (PEA)₂PbI₄ perovskite thin films, the photoexcited electrons are trapped by PCBM. As a result, the photocurrent response and the photocatalytic rate get reduced in PCBM mixed (PEA)₂PbI₄ perovskite thin films.

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Unraveling the Oxygen Reduction Reaction Activity under Acidic Medium Using Designed N-doped Graphene Catalyst

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Abstract

In the search of low-cost high performance oxygen reduction reaction (ORR) catalyst for the advancement and viability of the hydrogen fuel cell technology, the discovery of metal-free N-doped carbon materials have revolutionized the catalysis research. In addition, later studies revealed that the pyridinic-N (pyri-N) creates the O₂ adsorption site at the neighboring carbon.¹ The N-doped carbon materials have displayed a similar ORR activity to the state-of-the-art (Pt/C) catalyst under alkaline electrolyte (KOH). However, the origin of lower ORR activity under acidic medium (H₂SO₄/HClO₄) is still not clarified. Studies shows the role of bulkier counter anions and protonation of doped-N is mainly responsible for the lowering of activity by reducing the O₂ molecule's accessibility and adsorption energy reduction to the active sites.²

To understand the ORR mechanism under acidic medium, the development of N-doped carbon catalyst with uniform N-doping and well-defined structure is the primary requirement.³ In the present study, we have achieved a thin layer coating of cyanuric acid (N-precursor) functionalized (hydroxyethyl)methacrylate (HEMA) polymer over the graphene oxide (GO) by controlled U.V. polymerization. The uniformly distributed N-precursor over the GO layer was utilized for N-doping by high-temperature treatment resulting into the N-doped reduced graphene. The chemically N-doped graphene (cNrGO) achieved by following the controlled coating process has shown a superior catalytic activity ($E_{\text{onset}} = \sim 0.82$ V, $E_{1/2} = 0.61$ V (vs. RHE)) as compared to the physically mixed sample (pNrGO) ($E_{\text{onset}} = 0.52$ V, $E_{1/2} = 0.31$ V (vs. RHE)). Furthermore, the ORR catalytic pathway was confirmed by the DFT calculations using Vienna ab-initio simulation package (VASP), illustrating the role of protonation of doped-N towards the ORR activity alteration. In addition, the effect of spin density change due to N-doping is being verified by the EPR studies.

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Ionic Liquid Assisted Single Sodium-Ion Conducting Styrene-Maleic Anhydride Copolymer for Energy Storage Application

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Abstract

Presently a large amount of research has been done on “ionic liquid” (IL)¹ supported conducting polymers in energy storage devices². Herein, by taking the reaction advantage of styrene maleic anhydride (SMA) copolymer with sodium hydroxide, we synthesize a sodium ion having polymeric material as an electrolyte³. We use DBU Acetate as an IL synthesize by reaction of DBU and acetic acid and then added into the hydrolyzed SMA Copolymer to increase the matrix flexibility of electrolyte material and semi-solid nature, which allowed ions to move easily inside the matrix⁴. This sodium ion-based solid polymer electrolyte shows conductivity in the order of 10^{-5} S cm⁻¹, an electrochemical stability window of 2.52 volts with >97% of ionic transference. It also shows the diffusivity constant in the order of 10^{-4} m²/s and ionic mobility in order of 10^{-3} m² v⁻¹ s⁻¹ at 30°C temperature. The solid polymer electrolyte matrix shows a correlated type of hopping with a power exponent⁵.

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Hydrolysis-Mediated Hydrogen Production Using High Entropy Quintuple Alloy Grafted Carbon Black

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Abstract

Hydrogen is a promising fuel due to its sufficient energy density and carbon-free combustion. Its rapid and efficient production from hydrogen-rich compounds like sodium borohydride (NaBH₄) is of significant practical relevance. In this study, we introduce a novel quintuple high entropy alloy, CrMnFeCoNi, supported on conductive carbon (HEACB), as an efficient heterogeneous catalyst for the hydrolysis of NaBH₄ to generate hydrogen at room temperature. The best-performing HEACB exhibited an impressive turnover frequency (TOF) and a low activation energy (E_a). Mott-Schottky analysis demonstrated that the HEACB heterostructure behaves as an n-type semiconductor at the electrolyte interface, showing an optimal flat band potential during the reaction. Electrochemical analysis was performed to better understand the kinetic factors influencing the observed catalytic activity in the hydrolysis process. Overall, a strong correlation emerged from the chemical and electrochemical data. Density Functional Theory (DFT) was utilized to analyze the interaction of reaction intermediates and clarify the borohydride hydrolysis process.

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Enhancement of OER Activity of CuO_x on Incorporation of Lanthanides

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Abstract

Electrochemical water splitting has emerged as a pivotal technology in clean energy storage. Among its components, the oxygen evolution reaction (OER), the anodic half-cell reaction, holds significant interest due to its relatively sluggish kinetics compared to the hydrogen evolution reaction (HER), the cathodic half-cell reaction. Recent investigations have spotlighted the promising OER activity of monometallic copper oxides; notably, Cu₂O-Cu hybrid foams have exhibited a low OER overpotential of around 250 mV at 10 mA·cm⁻².^[1] The work by the Yeo group revealed the correlation of OER activity to the population of Cu^{III} species, which was detected via in-situ Raman spectroscopy.^[2]

This study investigates the effect of incorporating lanthanides (Ln) into the CuO_x lattice for oxygen evolution activity. For this, we synthesized Cu_{1-y}Ln_yO_x and conducted an exhaustive electrochemical characterization of the catalyst. We found that Cu_{1-y}Ln_yO_x showed enhanced OER activity compared to CuO_x. We discovered that this catalyst displayed lower tafel slopes and polarisation resistance than CuO_x, indicative of the former's improved charge transfer kinetics. In-situ Raman spectroscopy was employed to identify the active species during the OER process, revealing that Cu^{III} species is the active participant. We also demonstrated that incorporating Ln led to an increase in the population of Cu^{III} species, and the increase in Cu^{III} species population showed direct correlation with the enhanced OER activity.

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Electrocatalytic Performance of Mn-doped Cobalt Ferrites for Water Splitting Applications

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Abstract

Developing a low-cost, high-efficiency bifunctional electrocatalyst is essential for producing green energy. Herein the Mn doped cobalt ferrite (MCF) nanoparticles are synthesized and explored as bifunctional electrocatalyst for oxygen evolution reaction, hydrogen evolution reaction, and overall water splitting. The MCF nanoparticles with varying Mn doping concentrations are synthesized using the combustion method, wherein green fuel is employed as a fueling agent. This study compares the electrocatalytic activity of varying Mn doped MCF nanoparticles. $\text{Mn}_{0.5}\text{Co}_{0.5}\text{Fe}_2\text{O}_4$ (MCF 0.5) sample exhibited superior electrocatalytic performance with overpotentials 270 mV and -177 mV at 10 mA/cm² towards OER and HER, respectively. Furthermore, $\text{Mn}_{0.5}\text{Co}_{0.5}\text{Fe}_2\text{O}_4$ (MCF 0.5) demonstrated an impressive electrolysis cell voltage of 1.60 V at a current density of 10 mA/cm² with excellent long-term stability. The work proposed here offers a novel synthetic process for Mn doped cobalt ferrite nanoparticles which can be further successfully applied as a low-cost bifunctional electrocatalyst for overall water splitting.

Green Recycling and Regeneration of Carbon-coated LCO from Spent LIBs

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Abstract

Spent lithium-ion batteries (LIBs) are an excellent secondary resource of critical minerals such as lithium, cobalt, and nickel. Hence, it is imperative to process them in an environmentally friendly manner in order to extract and reuse critical minerals, as the innate heterogeneity among battery materials based on different chemistries makes the extent of recycling highly source-dependent¹. In this context, the development of the hydrometallurgical recycling process employing green reagents has been examined for a cobalt-rich spent LIB material by varying various parameters such as acid concentration, reducing agent dosage, and microwave power. The leaching operation was optimized to achieve leaching efficiencies of Li: 96.47 %, Co: 95.10 %, Ni: 94.80 % and Mn: ~100 %. Up to 90% of metal values were coprecipitated in the form of a metal-organic coordination complex, followed by further processing to regenerate carbon-coated lithium cobalt oxide (LCO) cathode. The regenerated carbon-coated LCO shows superior reversible discharge capacity and excellent rate capability. Furthermore, lithium was recovered as high-purity (~98%) lithium carbonate. The green route enables efficient recycling of spent LIB material, which paves a pathway for generating eco-friendly value-added products with high throughput processing towards a sustainable future.

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Anchoring Ni doped Mn_3O_4 on Bimetallic CoFe Layered Double Hydroxide for Efficient Electrocatalytic Oxygen Evolution Reaction

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Abstract

The advancement of highly effective electrocatalysts for water electrolysis applications has become a prominent topic of interest. In particular, the oxygen evolution reaction (OER) has garnered considerable attention due to the substantial overpotential associated with the intricate four-electron transfer coupled reaction. Developing two-dimensional, nonprecious, and durable electrocatalysts for oxygen evolution reactions (OERs) is crucial for advancing commercial water-splitting technology. Herein, we have constructed a 2D heterostructure Ni doped Mn_3O_4 /CoFe layered double hydroxides (LDH) mixed composite on a GCE substrate using a low temperature one-step co-precipitation synthesis method. The as-prepared Ni doped Mn_3O_4 /NiFe LDH (40 wt%) electrocatalyst drives a 10 mA/cm^2 OER with the lowest reported overpotential of 330 mV and a Tafel slope 38 mV/dec OER process in 1 MKOH electrolyte. These OER activities are superior to that of the state-of-the-art RuO_2 OER electrocatalyst. The excellent OER activity appears to be due to the synergetic effect of CoFe LDHs and Ni doped Mn_3O_4 . In addition, the presence of relatively non expensive Ni metal exhibits excellent corrosion resistance in alkaline medium and the Ni doped Mn_3O_4 /NiFe LDH composite sheets provides many active edge sites, which contributes to improving the electronic conductivity of the electrocatalyst.

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Detailed Electrochemical, Synchrotron and DFT Investigations into the Enhanced Solar Promoted Photocatalytic Mitigation of Chloramphenicol and H₂ Evolution by CuNi Alloy Bimetallic Nanoparticle Modified on h-BN Doped g-C₃N₄

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Abstract

A simple one-step deposition-precipitation method was used to synthesize CuNi alloy bimetallic nanoparticles supported on h-BN/g-C₃N₄. The nanocomposite was applied for hydrogen gas evolution and photocatalytic chloramphenicol (CHP) removal. Through TEM and synchrotron studies, formation of CuNi alloy and uniform distribution of CuNi bimetallic nanoparticles on the h-BN/g-C₃N₄ surface was observed^{1,2}. The EXAFS analysis verified successful formation of the alloy, while the XPS and XANES spectra showed that the bimetallic nanoparticles are in a metallic state^{3,4}. Additionally, XANES revealed nanoparticle distortion upon interaction with the support, confirming the effective formation of the nanocomposite. The nanocomposite achieved a maximum hydrogen evolution rate of 3658.9 $\mu\text{mol g}^{-1}\text{h}^{-1}$ for 5wt% CuNi(3:1)/h-BN/g-C₃N₄, outperforming CuNi(3:1) nanoparticles and pristine g-C₃N₄ by 1.82 and 4.31 times, respectively. Additionally, it degraded chloramphenicol with a rate constant (k_{app}) of 0.018 min^{-1} . Optical and electrochemical analysis revealed enhanced charge mobility, extended lifetime, improved photostability, and superior photoresponse. X-ray absorption spectroscopy (XAS) and Density Functional Theory (DFT) calculations attributed the performance to the synergy between the bimetallic nanoparticles and the h-BN/g-C₃N₄ sheet. DFT calculations demonstrated effective breakdown of chloramphenicol and promotion of hydrogen gas evolution, aligning with experimental observations⁵. Cytotoxicity of CHP post-treatment was analyzed using *Drosophila melanogaster* (fruit fly) and the Oregon-R strain of *Drosophila melanogaster*.

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Selective Electrochemical Nitrogen Reduction to Ammonia by an Organic-Inorganic Hybrid Microporous Vanadium Phosphonate Material via the Distal Mechanism

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Abstract

The primary industrial method for producing ammonia, a necessary chemical, is the labor- and capital-intensive Haber-Bosch process, which dates back a century. Hence, the electrochemical nitrogen reduction reaction (NRR), generating ammonia under ambient settings, is gaining much research interest. However, the overall NRR process suffers due to strong N≡N bond, low faradaic efficiency, and low adsorption propensity of the nitrogen molecule. This presents an intriguing challenge in the development of an efficient electrocatalyst for electrochemical NRR.¹⁻³ Herein, a microporous organic-inorganic hybrid vanadium phosphonate (VPn) material was synthesized by employing phenylphosphinic acid and vanadium chloride through a solvothermal reaction, without using any surfactants. Owing to its reasonable surface area and crystalline pore wall with regular microporous channels, VPn has been investigated as a potential NRR electrocatalyst. The maximum ammonia yield rate and maximum faradaic efficiency were 11.84 $\mu\text{g h}^{-1} \text{mg}_{\text{cat}}^{-1}$ at -0.6 V and 40.63% at -0.5 V respectively, as determined by the phenate method and 11.2 $\mu\text{g h}^{-1} \text{mg}_{\text{cat}}^{-1}$ at -0.6 V and 36.56% at -0.5 V respectively as estimated by indophenol blue method. DFT studies reveal distal pathway as the optimal route for electrochemical NRR, with the potential-determining step being the first protonation step of $^*\text{N}_2$ leading to $^*\text{NNH}$.⁴

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Gold Nanoparticles: Revolutionizing Bio-Electrolysis Efficiency

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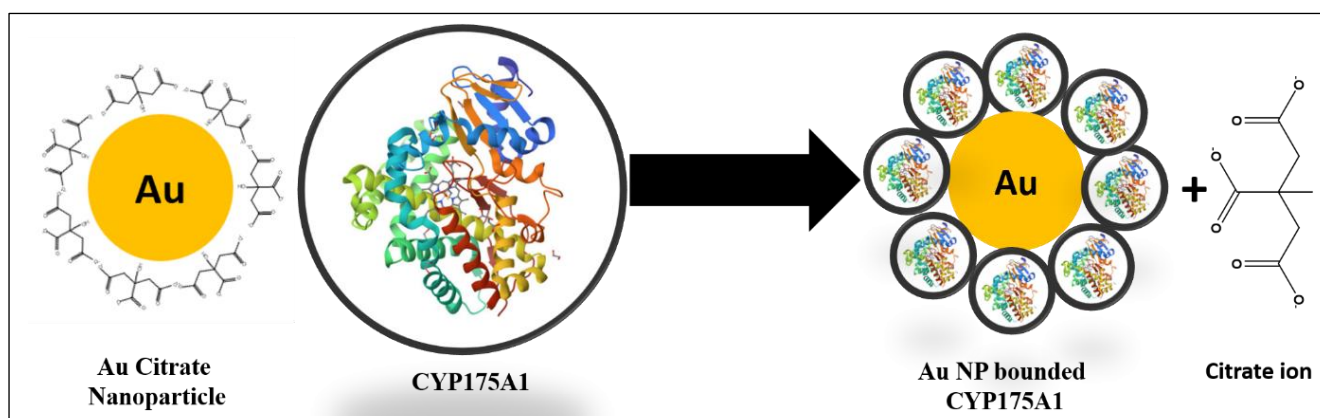
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Abstract

CYP175A1 is a Thermostable enzyme from the Cytochrome P450 superfamily, known for catalyzing the monooxygenation of organic substrates. However, CYP175A1 requires suitable electron transfer process coupled to the substrate binding for efficient enzymatic reaction of the substrate. In view of this, this enzyme exhibits low reactivity toward organic substrates because of inefficient electron transfer and substrate binding to the active site,^{1,2} requiring additional mutations at the active site to enhance catalytic activity. To improve its electrocatalytic activity, Gold nanoparticles (Au NP) are used to enhance electron transfer due to their excellent conductivity and high surface area for protein loading capacity without causing denaturation of the proteins.^{3,4}

In this study, freshly synthesized Au nanoparticles (Au NPs) were used to modify a gold electrode with cysteamine. The Au NP-modified electrode, along with CYP175A1, showed improved cyclic voltammetric response under both aerobic and anaerobic conditions. The surface coverage of Au nanoparticles was found to be 216 pMol/cm² and the reduction potential ($E_{1/2}$) about -300 mV vs Ag/AgCl using cyclic voltammetry (CV) under anaerobic conditions. In aerobic conditions, a reduction current is observed at -375 mV vs. Ag/AgCl. Comparative CV studies can be conducted with wild-type CYP175A1 and cysteine-functionalized surface mutants of CYP175A1 to evaluate their electrochemical performance. This modification facilitates the CYP175A1 catalytic activity leading to hydroxylation of 1-Methoxynaphthalene to form Russig's blue dye. The Michaelis-Menten constant (K_M) was calculated based on substrate concentration and catalytic current using Lineweaver-Burk plots. The Russig's blue product was analyzed using UV-Vis spectroscopy and ESI-MS.



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Mechanical Milling induced synthesis of $a_m\text{Zn/Co-ZIF-8}$ For Enhanced Electrochemical Water Splitting

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Abstract

Developing highly efficient and low-cost electrocatalyst for hydrogen and oxygen evolution reaction in alkaline media is essential for energy storage and conversion system. Herein, we report the mechanical milling approach for the synthesis of amorphous hetero-metal ($a_m\text{Zn}_{50}\text{Co}_{50}\text{ZIF-8}$) state by adding equimolar concentration of two isostructural ZnZIF-8 and CoZIF-8. $a_m\text{Zn}_{50}\text{Co}_{50}\text{ZIF-8}$ was further transformed to crystalline hetero-metal ($c_r\text{Zn}_{50}\text{Co}_{50}\text{ZIF-8}$) state by exposing 95% relative humidity (RH) in water or methanol vapor at 25 °C for 3 days. Unique heterometal structure and enhanced catalytic active surface area of $a_m\text{Zn}_{50}\text{Co}_{50}\text{ZIF-8}$ displayed excellent electrocatalytic activity toward both OER and HER with overpotential of 301 mV for OER and 437 mV for HER at 10 mA cm⁻² current density in 1 M KOH. $a_m\text{Zn}_{50}\text{Co}_{50}\text{ZIF-8}$ showed enhanced electrocatalytic activity compared to their crystalline heterometal state, $c_r\text{Zn}_{50}\text{Co}_{50}\text{ZIF-8}$, amorphous (a) and parental (p) state of Zn/Co-ZIF-8.

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Metal Oxide Functionalized Hollow Carbon Spheres as Electrocatalysts for CO₂ Reduction

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Abstract

Development of novel electro-catalytic materials based on hollow carbon spheres (HCSs) is an emerging area of interest for addressing the drawbacks of conventional electrocatalysts such as sluggish reaction kinetics, inadequate selectivity, and poor stability.¹ These carbon materials are also promising due to their tailorable porous structures, resistance to acids and bases, high-temperature stability, and environmental friendliness.² Adoption of suitable functionalization strategies (nonmetal doping, metal single-atom anchoring, and metal nanoparticle modification) for HCSs can boost the performance of the electrocatalyst due to synergistic effects.

In this work, functionalization of the various HCSs with various metals / metal oxides was performed and evaluated for their electrochemical CO₂ conversion efficiency.³ Due to the mechanistic intervention of the metal and improved selectivity provided by the HCSs, one can achieve higher faradaic efficiency of a specific product.⁴ The electrodes were characterized using advanced analytical techniques like XRD, XPS and Raman. The performance evaluation of the electrodes were studied using three electrode system. Polarization studies like CV and CA have been performed and the reaction was monitored for various products like methanol and formic acid by using NMR technique.

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Atmospheric Pressure Plasma Surface Modified Separator for Lithium Ion Battery

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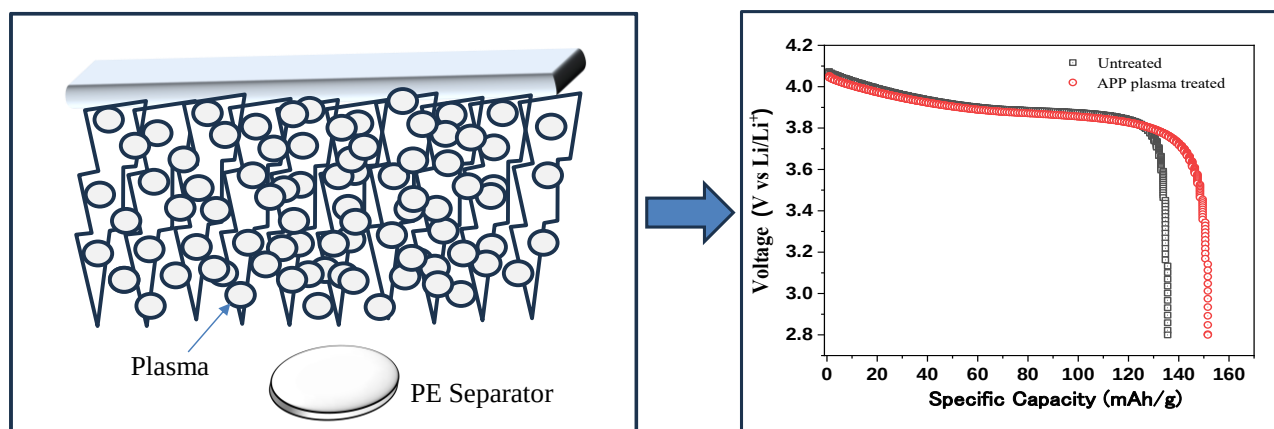
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Abstract

Separator is an important component of the lithium-ion battery (LIBs), which strongly influence life, performance and safety of the cell. The Polyolefin based commercial separators available in the market such as polyethylene (PE) and polypropylene (PP) exhibit poor wettability and electrolyte retention. Apart from various methods reported in the past [1-5] to overcome these drawbacks, atmosphere pressure plasma (APP) treatment is simple, fast, cost-effective, environmentally benign, and low temperature dry process for surface modification of the separator.

In this study, APP assisted surface modification on the PE separator was carried out and electrolyte uptake, morphology and electrochemical properties of the separators have been reported. LCO/Li cells without and with plasma treated separators showed the initial discharge capacities of 135.60 and 151.31 mAh/g, respectively at a 0.1C rate. The plasma treated PE separator showed a higher capacity retention value (39.82%) than the cell with untreated PE separator (27.43%) after 50 cycles at a 0.1 C-rate. The enhanced performance of plasma treated separator was probably due to the improved compatibility with the organic electrolyte and its higher affinity towards electrodes. These results demonstrate a high potential of the plasma-treated PE separator in LIBs



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High-Performance Symmetric Dual-Carbon Lithium-Ion Capacitor with Graphitized and Activated Carbon Xerogel Electrodes

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Abstract

The design of symmetric electrodes is crucial for balancing the energy and power densities of lithium-ion capacitors (LIC). In the present work, we synthesized anode and cathode materials for dual carbon LIC using the same resorcinol-formaldehyde xerogel (RFX) as a carbon precursor. To facilitate intercalation in anode, the presence of graphitic domains is essential. To achieve this, we catalytically graphitized RFX using Fe and Co catalyst (AFCRFX) at a moderate temperature of 1100 °C. While for the cathode, we activated the same precursor, RFX, resulting activated RFX (ARFX) with specific surface area (SSA) of 1182 m² g⁻¹, with a dominance of micropores, making it suitable for a capacitive electrode. The prelithiated AFCRFX anode and ARFX cathode in the full cell with a 1:2 mass configuration demonstrated a high specific capacitance of 171.4 F g⁻¹ at 0.2 A g⁻¹. This system exhibited a high energy density of 117 Wh kg⁻¹ at a power density of 194 W kg⁻¹ and retained a capacitance of 75% for 5000 cycles at 1A g⁻¹. Furthermore, the mechanistic behavior of LIC was investigated below and above open circuit voltage to analyse diffusion and absorptive contribution to performance.

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Prudently Designed Se@fMWCNT as Peroxidase Mimicking Nanozyme for Distinctive Electrochemical Detection of H₂O₂ and Glutathione

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Abstract:

Nanozymes are nanomaterials with enzymatic characteristics that are employed to overcome the challenges associated with the naturally occurring enzymes. A peroxidase mimicking nanozyme has been developed in this work which has the ability towards reduction of hydrogen peroxide (H₂O₂) to water, by oxidising the substrates in the presence of H₂O₂. We have designed and developed a neoteric Se@fMWCNT nanocomposite with peroxidase mimicking activity towards electrochemical detection of H₂O₂ and glutathione (GSH). The choice of selenium (Se) was inspired from the natural enzymatic antioxidant, glutathione peroxidase, which consists of Se as its active metal centre. Prior to preparation of nanocomposite, MWCNT was functionalized with acid to obtain fMWCNT in order to improve biocompatibility and to increase conductivity by providing abundant active sites for the successful incorporation of Se. The as-synthesized nanocomposite was immobilized on the glassy carbon electrode using which analytes H₂O₂ and GSH were detected amperometrically at neutral pH. The fabricated sensor portrays a linear range of 50 nM – 1.4 μM and a limit of detection (LOD) of 18.23 nM for H₂O₂, and linear ranges from 50 - 450 μM and 500 μM – 1.5 mM during GSH determination with a LOD of 19.2 μM for GSH.

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Nitrogen-Doped Ti_3C_2 MXene Quantum Dots/ MoSe_2 Heterostructure: A New Avenue for Efficient Water Splitting

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Abstract

The emerging family of two-dimensional (2D) materials, especially MXene, has gained significant attention in scientific research due to its outstanding properties like high electrical conductivity, excellent thermal performance, and strong mechanical strength.¹ In this study, we successfully constructed a new heterostructure by combining nitrogen-doped Ti_3C_2 MXene quantum dots (N-MQD) with MoSe_2 using a solvothermal method for water-splitting applications.² Nitrogen doping enhances the electronic properties of the MXene quantum dots, leading to improved catalytic activity.³ When these N-MQD are combined with MoSe_2 , a well-known layered material, the resulting heterostructure exhibits a synergistic effect that significantly enhances both the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), in water splitting.⁴ Our results indicate that the N-MQD/ MoSe_2 heterostructures exhibit remarkable electrocatalytic performance, with significantly improved efficiency compared to undoped MXene quantum dots (MQD) and MoSe_2 alone. This work opens a new avenue for designing advanced, cost-effective catalysts for hydrogen production, offering a promising route toward practical and scalable water-splitting systems. The findings may pave the way for further exploration of MXene quantum dot-based materials in renewable energy applications.

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Evidence of bimetallic cooperativity in water oxidation catalysis: The Key Role of Second Metal

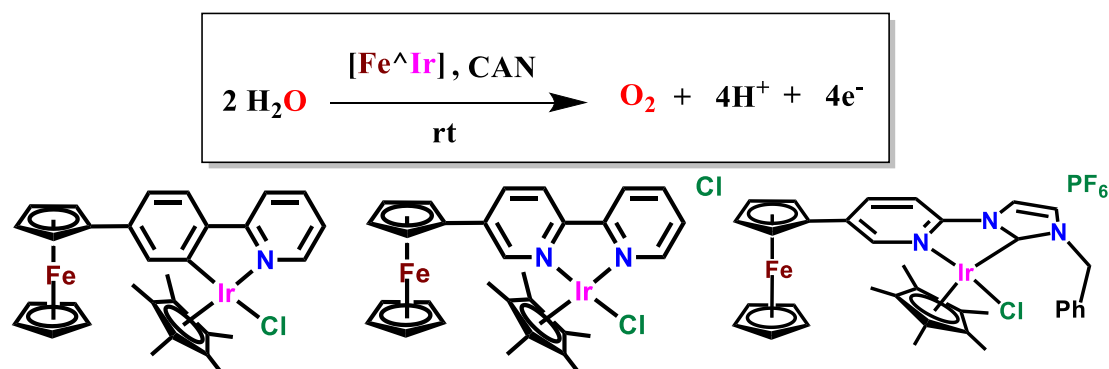
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Abstract

A key challenge for scientists today is strengthening sustainable methods for the production of green fuel. Our reliance on fossil fuels has driven up CO₂ levels, intensifying global warming. This pinnacles the urgency for innovative technologies harnessing renewable energy by paving the way toward a cleaner and greener future. Artificial photosynthesis, inspired by nature's brilliance, shines as a beacon of hope for clean energy. By transforming sunlight, water, and CO₂ into carbohydrates and oxygen, it mimics the remarkable efficiency of plants. Researchers across the globe are aspiring to replicate this process in laboratories, with water splitting producing solar fuel ($2\text{H}_2\text{O} \rightarrow \text{O}_2 + 4\text{e}^- + 4\text{H}^+$; $2\text{H}^+ + 2\text{e}^- \rightarrow \text{H}_2$) emerging as one of the most vital reactions in artificial photosynthesis.¹ Presently, molecular catalysts offer an encouraging solution to accelerate water oxidation, a crucial step in water splitting. Bimetallic [Fe^{II}/Ir^{III}] complexes have been synthesized and characterized using techniques like NMR, HRMS, CV, and SCXRD.² These catalysts efficiently generate oxygen from water with ceric ammonium nitrate (CAN) as the oxidant.³ High TON and TOF are obtained with these bimetallic catalysts. Synergistic bimetallic cooperation of iron (Fe) and iridium (Ir) are the main reason behind such activities which are established during mechanism studies. This will be discussed elaborately.



Water oxidation reaction by bimetallic [Fe^{II}/Ir^{III}] catalysts.

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Synergistic Effects of Nitrogen and Sulfur Co-doping in Xerogel Derived Hard Carbon for High-Performance Lithium-Sulfur Batteries

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Abstract

Lithium-sulfur battery (LSB) is a promising future candidate for fulfilling the high energy demands for electric vehicles and aerospace applications. However, its commercialization is hindered by the insulating sulfur, volume changes, and the polysulfide shuttling effects. In this work, we reported a dual heteroatom-doped resorcinol-formaldehyde xerogel-derived hard carbon (NSRFC) as a cathode host. The scalable one-pot synthesis paves the way for developing an efficient cathode matrix for future applications. The physicochemical characterizations confirm the successful incorporation of heteroatoms in the carbon framework and the development of the sulfur host with adequate surface area and graphitic domains. It helps trap the polysulfides, enhance the electronic conductivity, and accommodate the volume changes. The electrochemical studies further validate the cathode matrix's efficiency in enhancing performance with long cyclability and excellent capacity retention. The cell with a high aerial loading cathode delivers an initial discharge capacity of 1170 mAh g⁻¹ at 0.1 C and a capacity of 667 mAh g⁻¹ after 500 cycles at 1.0 C with excellent capacity retention. The results confirm the advantage of NSRFC in boosting the performance of the LSB, and the scalable one-pot synthesis approach paves the way for developing the cathode host for commercial applications.

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Re-nucleation and re-precipitation in Soluble Lead Redox Flow Battery

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Abstract

The membrane-less soluble lead redox flow chemistry with high energy (~70%) and coulombic (~90%) efficiencies [1] is restricted from commercialization as a cost-effective large-scale energy storage device due to its poor cyclability (best reported about 100 cycles [2]) attributed to the accumulation of PbO_2 deposits, which shed over cycling, causing an irrecoverable loss of active species from the electrolyte.

We seek to unravel residue build-up by analyzing two unexplained but universal features of this chemistry's charge-discharge characteristics: (i) potential peak at the resumption of charging and (ii) potential dip at the start of discharge. We show that this potential peak is an intrinsic feature of any charging following a discharge, distinct from the peak due to charging a fresh electrode and is independent of the discharge duration. Through SEM images, we propose these peaks represent the recursive nucleation of solid PbO_2 on an electrode with a residual deposit, forming a layered structure prone to cracking and flaking. On the other hand, the potential dip at the discharge onset could be attributed to an analogous established characteristic observed during discharge in the classical lead acid battery [3,4] through the 'dissolution-precipitation' mechanism, which explains the residue formation in the first place.

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Exploring the Electrocatalytic Superiority of Cobalt and Iron based Precatalytic Oxalate Framework towards Alkaline Water Oxidation

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Abstract

To implement carbon free sustainable energy usage, hydrogen fuel has become an utmost choice due to its several advantages¹. However, to mitigate the sluggish oxygen evolution kinetics², an efficient catalyst with abundant active sites and better catalytic proficiency is needed. In this work, we synthesized an iron-incorporated cobalt-based oxalate framework ($\text{CoC}_2\text{O}_4/\text{FeC}_2\text{O}_4$) via a simple one-pot co-precipitation technique.³⁻⁴ The as-prepared composite showed enhanced OER activity, delivering the benchmark current density (10 mA/cm^2) at 292 mV overpotential with improved intrinsic activity, higher turnover frequency, and durability. The enhanced activity can be attributed to i) the synergistic effect between cobalt and iron⁵, ii) improved per-site activity, and iii) increased active site density due to iron incorporation. Further, an HER catalyst cobalt selenide ($\text{Co}_{0.85}\text{Se}$) was synthesized⁶ using cobalt oxalate as a precursor, which required only 141 mV overpotential to reach the benchmark current density (-10 mA/cm^2). Finally, an alkaline electrolyser was constructed with cobalt-iron oxalate as anode and cobalt selenide as cathode, which required 1.68 V cell voltage to reach 10 mA/cm^2 , with 36 hours of excellent stability. The overall strategy unlocks a simple preparative method without any precious elements for real-world implementation.

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Manipulation of Interfacial Electronic Structure of NiFe LDH/Ni₃S₂ Heterostructure for Corrosion Resistant Sustainable Seawater Electrolysis

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Abstract

Design of heterostructure interfaces are considered to be beneficial for green hydrogen production by seawater electrolysis due to their electronic structure regulation and rapid charge transfer at interfaces.^{1,2} However, considering challenging chloride corrosion during seawater electrolysis, rational design of heterointerfaces with chloride retardation ability is desirable and interesting to explore.³ Herein, we developed NiFe LDH/Ni₃S₂ heterointerface, which has been found to be not only anodically active exhibiting overpotential of only 216 and 270 mV at 10 and 100 mA cm⁻² current densities but also sustainable over long hours in alkaline real seawater. The electrocatalyst showed excellent corrosion resistivity and robust stability at high current density of 500 mA cm⁻² over 100 h in alkaline seawater. Additionally, the heterostructure combination also showcased optimal HER response, which leads to achieve a great overall performance by reaching 500 mA cm⁻² current density at a cell voltage of only 2.0 V. The intercalated carbonate ions in NiFe LDH and *in-situ* formation of sulfate layers on NiFe-LDH/Ni₃S₂ played a crucial role in repelling chloride ions selectively, thereby protecting anode material during seawater electrolysis.^{4,5} Certainly, the work is believed to have much potential to pave a fruitful way for future hydrogen generation from seawater.

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Bimetallic Alloy Nanoparticle Embedded N-Doped Carbon Nanotube for Electrocatalysis and Zn-Air Batteries

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Abstract

Cobalt-nickel bimetallic alloy nanoparticles embedded N-doped carbon nanotube, synthesized via a facile in situ single-step method, developed for an application as electrocatalysts for oxygen evolution, oxygen reduction reaction, and rechargeable zinc-air battery. The different nitrogen moieties associated with carbon nanotubes modify the surface to design a unique architecture and strategy for robust performance in harsh environments. Incorporation of nitrogen in nanotube creates the defective porous carbon framework, enhancing the surface area and porosity, which exposes the large active centers for catalytic reactions. The results showed that the best synthesis conditions of cobalt-nickel nanoparticle-embedded N-doped carbon catalysts improves the electrical conductivity and reduces the ions diffusion path; therefore, it reflects on the result as exhibiting a low overpotential, minimum activation energy, large ECSA and excellent stability in aq. 0.1M KOH alkaline media for OER. Furthermore, our results show an opportunity for multifunctional catalyst, efficient, and durable electrocatalysts for a low cost and scalable production for the rechargeable zinc-air battery.

Overcoming Activity-Stability Tradeoff in Water Splitting Catalysis: Lower Overpotential and Higher Stability of Ni-doped MoO₃ for Alkaline Oxygen Evolution

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Abstract

Electrochemical water splitting using earth-abundant materials is a crucial endeavor for enabling green hydrogen production and energy storage.^{1,2} In recent years, MoO₃ has been proposed as a candidate catalyst for the oxygen evolution reaction (OER).^{3–7} Here, we advance nickel doping of MoO₃ as a strategy to increase the activity and stability of the material, thereby overcoming the typical activity-stability tradeoff encountered with OER catalysts. Using density functional theory calculations incorporating Hubbard corrections to model localized electrons. We show that Ni-doping leads to a comparatively lower thermodynamic OER overpotential of 0.64 V on the MoO₃. Experiments demonstrate that Ni-doped MoO₃ requires an overpotential of 0.34 V for a current density of 10 mA/cm², as opposed to a value of 0.40 V for pure MoO₃. Further, Ni-doped MoO₃ exhibits a lower Tafel slope of 74.8 mV/dec, as compared to 98.3 mV/dec for the pristine material under alkaline conditions. While Mo leaches into alkaline conditions, an aspect missed by previous studies, we show using X-ray photoelectron spectroscopy that Ni-doping increases the stability of MoO₃ under alkaline conditions. Overall, our work reveals Ni-doped MoO₃ as a promising electrocatalyst and provides new insights into its OER mechanism, as well as its stability in alkaline media.

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Engineering MXenes to Boost their Performance in Batteries

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Abstract

Discovered in 2011, MXenes are a family of two-dimensional, 2D, transition metal carbides, nitrides, and carbonitrides¹. Currently, there are over 30 distinct MXene compositions and structures with new ones being discovered regularly. MXenes are hydrophilic and behave as “conductive clays”, or “2D metals”, a hitherto unknown combination. Because of their ease of synthesis and unique combination of properties MXenes have shown a lot of promise in applications like EMI shielding, energy storage, gas sensing, water purification, hydrogen storage, and as a catalyst for hydrogen evolution reactions among numerous others. Considering just the field of energy storage MXenes have shown appreciable performance as high-capacity anodes for lithium, sodium, potassium, aluminum ion batteries, and even supercapacitors.

In this talk, I will focus on how we can engineer MXenes during or post-synthesis to improve various aspects of their performance in battery electrodes. I will discuss in detail how various parameters like the architecture of MXene sheets, the solvent used during synthesis, the method of synthesis, and the interlayer space between the MXenes flakes affect its electrochemical performance. Finally, I will briefly discuss how MXenes can also be used as conductive additives in other battery chemistries like Sulfur batteries.²⁻⁴

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N-doped Norbornane sp^2 Carbon Framework: An Efficient Electrocatalyst for Oxygen Reduction and Hydrogen Evolution Reaction

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Abstract

At present, the development of Pt-free bifunctional electrocatalysts for energy conversion reactions like oxygen reduction reaction (ORR), and hydrogen-oxygen evolution reaction (HER=OER) are necessary for the advancement of sustainable and cost-effective solutions for energy conversion and storage technology. In this direction, herein we report N-doped sp^2 hybridized carbon framework (N-CF) as a metal-free electrocatalyst for ORR and HER. This work inspects the effect of N doping that converts a hybrid structure of CF {Norbornane or bicyclo [2, 2, 1] heptane structure} into planar N-CF. A series of N-doped CF with different doping concentrations has been prepared using a facile and cost-effective technique. These robust electrocatalysts exhibit a promotional effect on the activity, porosity, and thermal and electrochemical stability of the ORR and HER reactions. A rich delocalized electronic density of the sp^2 -bounded N species helps in modulating the antibonding state of molecular oxygen and facilitates the breakage of the O=O bond in ORR. It also promotes proton adsorption via bonding between proton and valence electron-rich catalyst surface to aid HER. The research sought to investigate the employability of N-CF for fabricating sustainable energy devices with electrocatalysts possessing multiple electrocatalytic activities for ORR and HER.

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Fabrication and Characterization of Functionalized Metal-Organic Framework Embedded Proton Exchange Membranes for Green Hydrogen Production in PEM Water Electrolyzer

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Abstract

In this study, the initial step involved the synthesis of a proton exchange membrane (sulfonated polyether ether ketone (SPEEK)) and Sulfonated Zr-MOF808. Subsequently, the performance of the SPEEK polymer was enhanced by incorporating sulfonated Zr-MOF808. Incorporating sulphonated Zr-MOF nanoparticles, the suitable sulfonating site (fixed negative charges) in SPEEK polymer will increase. Characterization of Cation Exchange Membranes SPEEK and nano-composite polymer (SZM/SPEEK) was conducted including Water Uptake %, Membrane Swelling%, TGA, Tensile Strength, ¹H NMR, Contact Angle, FESEM, Membrane Conductivity (EIS), Ion Exchange Capacity (IEC), Current-Voltage (I-V) relations, Hydrogen production Rate, Gas Chromatography (GC) etc. There was an enhancement of the -SO₃H active sites within the membrane, which helps in enhancing the H⁺ path in the membrane thus formation of Stable Membrane Electrode Assembly (MEA) and we can use in other applications includes Hydrogen Fuel Cell, electrodialysis etc. This work will surely contribute towards sustainable development of our Earth.

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Nickel-Embedded Carbon Nanostructures as Noble Metal-Free Catalysts for the Hydrogen Evolution Reaction

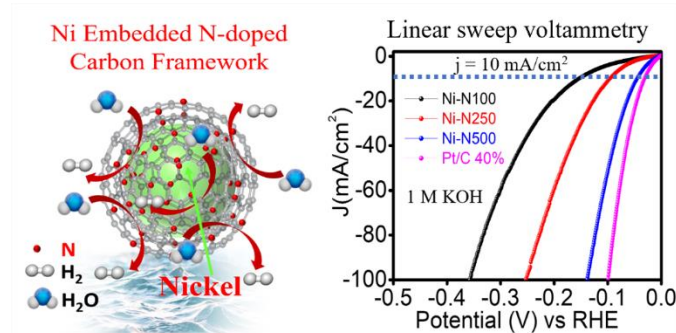
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Abstract

We demonstrate the electrocatalytic activity of “nitrogen (N)-doped porous carbon matrix embedded with nickel nanoparticles” for efficient hydrogen evolution reaction (HER) in alkaline medium. Three samples were synthesized via pyrolysis of a fixed amount of Ni(acac)₂, along with three different amounts of nitrogen precursor melamine (100, 250, and 500 mg) separately. The varying nitrogen concentrations of the surrounding carbon layers on the Ni nanoparticles enhance the surface area and porosity, exposing extensive active sites for catalytic reactions. The transition metal-based catalysts are crucial for long-term sustainability due to their combined edge (effectiveness and inexpensiveness) over traditional catalysts. Thus, by employing the protective carbon layer on the transition metal nanoparticles, we fabricated a catalyst that exhibits outstanding performance, with a low overpotential of 45.6 mV at 10 mA cm⁻² in 1 M KOH and maintains it for 24 h (durability), highlighting its exceptional catalytic efficacy and stability. The pores in carbon nanostructures facilitate the ionic moieties to move to active sites inside the pores. As the pore size variation influences the movement of charge or diffusion, this is reflected in the magnitude of impedance ($|Z|_{\text{imp}}$). Consequently, the enhanced number of active sites along with the larger pore sizes resulting from optimum amounts of nitrogen doping enables the sample with minimal $|Z|_{\text{imp}}$ and an enhanced HER performance. The present study demonstrates the way to design a sustainable, extremely effective, and inexpensive HER electrocatalyst¹.



Graphical abstract

Reference

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Electronic Redistribution through the Interface of MnCo_2O_4 – Ni_3N Nano-Urchins Prompts Rapid in Situ Phase Transformation for Enhanced Oxygen Evolution Reaction

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Abstract

This work describes the in situ electrochemical phase transformation of MnCo_2O_4 – Ni_3N into MnCo_2O_4 – NiOOH . The catalyst has an exceptional overpotential of 224 mV to drive a current density of 10 mA cm^{-2} . Strong interfacial contact is seen in the MnCo_2O_4 – Ni_3N catalyst, leading to a considerable electronic redistribution between the MnCo_2O_4 and Ni_3N phases. This causes an increase in the valence state of Ni, which makes it an active site for the adsorption of $^*\text{OH}$, O^* and $^*\text{OOH}$ (intermediates). This charge transfer facilitates the rapid phase transformation to form NiOOH from Ni_3N . At a higher current density of 300 mA cm^{-2} , the catalyst remained stable for 140 h. DFT studies also revealed that the in situ-formed NiOOH on the MnCo_2O_4 surface results in superior OER kinetics compared to NiOOH alone.

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Ruthenium Nanoparticles onto MXene through “Defect Engineering” to Enhance the Activity of the Hydrogen Evolution Reaction in Alkaline medium

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Abstract

To enable large-scale implementation of the hydrogen evolution reaction (HER) in alkaline water splitting, the development of cost-effective, highly active, and durable electrocatalysts is essential. While non-precious metal electrocatalysts often fall short of the performance of platinum, in this study, we synthesized ruthenium (Ru) nanoparticles on both pristine MXene and defect-rich MXene (d-MXene), with ultra-low ruthenium (average particle size 2.2 nm) loading to enhance atom utilization efficiency on the defect-enriched MXene. The Ru nanoparticles were primarily deposited on the molybdenum vacancies of the defect MXene. Our comparative analysis revealed that the Ru nanoparticles on d-MXene achieved an over-potential of 190 mV at a current density of 100 mA/cm², whereas the pristine MXene sample required 237 mV to reach the same current density. Additionally, chronoamperometry tests showed that the d-Ru-MXene sample maintained a stable current density of 63 mA/cm² over 20 h during long-term stability assessments. We also evaluated the Faradaic efficiency of four samples: MXene, d-MXene, Ru-d-MXene, and Ru-MXene. Among these, the ruthenium-decorated d-MXene exhibited the highest Faradaic efficiency of about 84%. Our work meticulously shows the defect-metal support interaction as an excellent strategy for achieving alkaline HER with a high Faradaic yield.

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Lattice Engineering Triggered Phase Formation of Bimetallic Thiospinels with Excellent HzOR Activity for Energy-Efficient Hydrogen Production

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Abstract

Introduction of foreign elements into a crystal lattice can trigger phase transformation, providing an excellent way to fabricate desired phases with enhanced electrocatalytic activity. NiCo₂S₄ is a well-known phase, generally synthesized via two-step synthesis route, and recognized as a good catalyst for multiple electrocatalytic reactions. However, pure phase NiCo₂S₄ is rarely explored in the case of electrocatalytic hydrazine oxidation reaction (HzOR). In this work, we report one-step syntheses of bimetallic thiospinels NiCo₂S₄ and CuCo₂S₄ by cation incorporation of Ni/Cu in Co₉S₈ system and their catalytic performance for HzOR. To study the growth mechanism, time-dependent syntheses were done, which suggested initial formation of (M, Co)₉S₈; M=Ni/Cu phase and subsequent conversion to thiospinel phases. Computational study validates that Ni incorporation into the Co₉S₈ system disrupts its stability and causes more stable thiospinel formation. The as-synthesized NiCo₂S₄ displayed remarkable activity for HzOR requiring only a potential of 350 mV to afford an industrial-level current density (500 mA/cm²) and showed excellent durability for 15 h. The two-electrode setup with NiCo₂S₄ as anode only required a potential of 140 mV to attain a current density of 10 mA/cm² for hydrazine-assisted H₂ production which is 1.39 V less than that required for conventional water electrolyzer (1.53 V).

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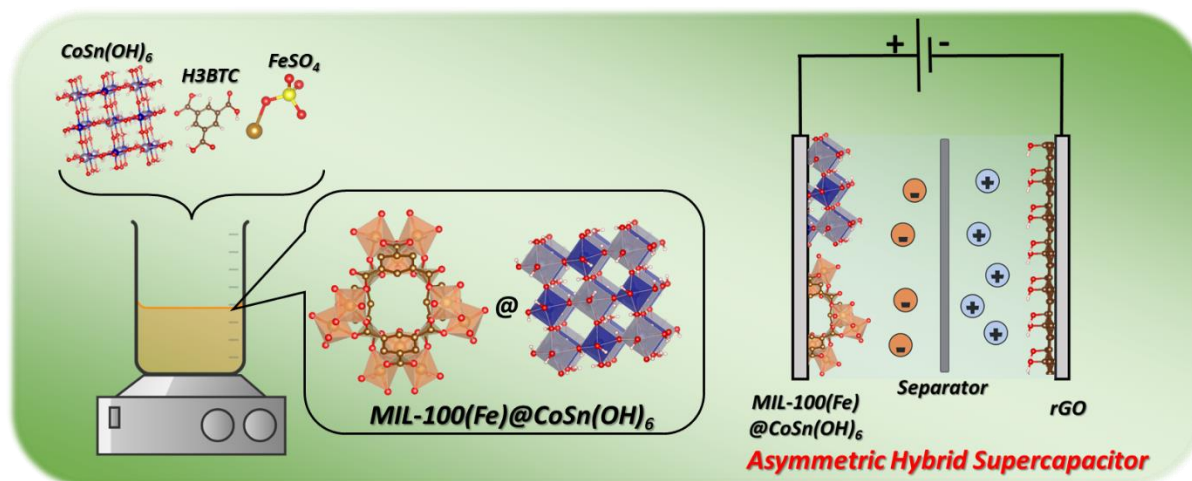
Investigating Electrochemical Performance of MIL-100(Fe)@CoSn(OH)₆ for Asymmetric Hybrid Supercapacitor

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Abstract

Supercapacitors have drawn a lot of attention due to their excellent electrochemical performance, longer cycling life, excellent specific power, and quick charging–discharging rates, but still the energy density and specific capacity of the supercapacitor are low compared to batteries. MOFs have gained attention as potential high-energy density electrode materials for supercapacitors due to their unique properties, including high surface area, tunable pore size and low density [1]. Here, we synthesized Fe-based MOF MIL-100(Fe) by a straightforward and scalable chemical approach without the need for hydrothermal or HF addition. The prepared MIL-100(Fe) conductivity was improved by the addition of cubic perovskite hydroxide CoSn(OH)₆ during the synthesis of MIL-100(Fe). This synthesized octahedral @ cubic MIL-100(Fe)@ CoSn(OH)₆ physical properties were studied using X-ray diffraction (XRD), scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS). The electrochemical performance of MIL-100(Fe)@ CoSn(OH)₆ was studied using cyclic voltammetry (CV), galvanostatic charge discharge (GCD), and Electrochemical impedance spectroscopy (EIS). Besides, the performance of asymmetric hybrid supercapacitor using MIL-100(Fe)@ CoSn(OH)₆ as a positive electrode and reduced graphene oxide (rGO) as a negative electrode is evaluated. This work suggests that MIL-100(Fe)@ CoSn(OH)₆/rGO is a promising configuration suitable for high-performance asymmetric hybrid supercapacitor applications.



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Effect of pH on hydrogen production from formic acid and study of role of Pd based catalysts

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Abstract

The decomposition of liquid formic acid (FA) is a promising method for on-site hydrogen (H_2) production. Studies show that maximum H_2 production occurs at a pH of 3.5 near the pKa of formic acid (3.75).^{1,2} Although supported palladium (Pd)-based catalysts have been widely studied, the effects of pH and the behaviour of these catalysts upon the addition of promoters like silver (Ag) remain underexplored.³ We investigated the effects of pH and metal-support interactions on monometallic Pd catalysts (Pd-CeO₂, Pd-TiO₂, and Pd-Al₂O₃) and bimetallic catalysts (Pd-Ag-CeO₂, Pd-Ag-TiO₂, and Pd-Ag-Al₂O₃) during H_2 production from FA at ambient temperature (25°C). The catalysts were prepared using incipient wetness impregnation method and the reaction was carried out in a batch reactor for 1 hr. Pd-CeO₂ provides a maximum rate of 6.82 mol H_2 (mol Pd)⁻¹ hr⁻¹ at pH 6, Pd-TiO₂ provides a maximum rate of 15.41 mol H_2 (mol Pd)⁻¹ hr⁻¹ at pH 6, while Pd-Al₂O₃ showed a maximum rate of 14.15 mol H_2 (mol Pd)⁻¹ hr⁻¹ at pH 4. These results highlight the role of support at different pH in formate activation which is different from the pKa of FA. Significant pH changes were also observed near pH 6 after catalyst addition, indicating interactions between the catalyst and the reaction medium.

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High Entropy Oxide towards Electrochemical Oxygen Evolution Reaction

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Abstract

RuO₂ and IrO₂ are two most extensively used electrocatalyst for OER¹, but in recent years, high entropy materials have grabbed much attention among researchers as a promising alternative OER catalyst for water splitting. High-entropy nanomaterial components can lead to extremely disordered structures and unsaturated coordination, which can produce more defects and promote the formation of more active metal sites for catalysis². Recently, we have synthesized a series of high entropy oxides (HEOs) of (FeNiCoCrMn)₃O₄ by one pot synthesis with a mixture containing different metals followed by varying their calcination temperatures from 600 °C-900 °C and also explored their OER activity³. Among all HEOs, HEO-700 have shown good catalytic performance with overpotential of 368 mV at a current density of 10 mA cm⁻² and the Tafel slope of 101.76 mV dec⁻¹ toward OER in 1.0 M KOH electrolyte. The morphological and structural properties of the synthesized HEOs were characterized via X-ray diffraction (XRD), Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM), X-ray Photoelectron Spectroscopy (XPS), Raman Spectroscopy, EXAFS (Extended X-ray Absorption Fine Structure). Besides that, we have also evaluated and compared the OER activity for HEO to those of the lower entropy oxides ranging from binary to quinary in alkaline electrolyte.

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NiSe₂@M(Cu, Al, Zn) doped NiCo-LDH as Efficient Electrocatalyst for Oxidation of 5-hydroxymethylfurfural

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Abstract

Biomass has the potential to produce a wide range of high-value chemicals and fuels¹ to replace fossil fuel-derived chemicals. 5-hydroxymethylfurfural (HMF) is one of the important platform chemicals derived from biomass, which is used to synthesise bio-based monomers such as 2,5-furandicarboxylic acid (FDCA). The development of noble-metal-free and durable electrocatalysts is crucial for the environmentally friendly conversion of biomass-derived HMF into FDCA. Nickel and Cobalt-based layered double hydroxide² (NiCo-LDH) catalysts have shown enhanced catalytic activity due to their adaptable layered structure and chemical compatibility. However, they suffer from low conductivity, which limits their performance. Electrochemical conductivity and catalytic activity can be improved by forming heterojunction³⁻⁴ using metal chalcogenides. Herein, nickel selenide (NiSe₂) at aluminium (Al), zinc (Zn) or copper (Cu) doped nickel cobalt layered double hydroxide (NiCo-LDH) on nickel foam as substrate was synthesised. Compared to NiCo-LDH, the nickel selenide formation leads to significantly enhanced performance in a divided cell and 3-D printed flow electrolyser. The parameters were further optimised by conducting an in-depth analysis of various reaction parameters, for instance pH, feed concentration, and applied potential using Raman and HPLC analysis.

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Highly efficient Mo doped CuNiFe based Metal Organic Framework (MOF) catalyst for overall water splitting application

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Abstract

MOF-based materials are crucial to the development and use of clean fuel hydrogen energy since they are bifunctional catalysts for electrocatalytic water splitting. Herein, We have synthesized the Mo doped CuNiFe based MOF using hydrothermal method and studied their electrochemical performance. The optimized MOF based electrocatalyst shows oxygen evolution reaction (OER) overpotential of 190 mV@10 mA/cm² and hydrogen evolution reaction (HER) overpotential of 50 mV@10 mA/cm² in 1M KOH solution. Furthermore, a full water-splitting electrolyzer consisting of a bifunctional Mo doped CuNiFe catalyst required a low cell voltage of 1.42 V to attain a current density of 10 mA/cm² with excellent stability for more than 50 h. This catalytic performance of Mo doped CuNiFe –MOF material can be assigned to the synergistic effect between transition metals and MOF with a tunable structure which result in an increased reaction rate due to the acceleration of charge and mass transfers. Thus, the present work introduces an efficient noble-metal-free electrocatalyst for clean hydrogen energy generation.

Keywords: Metal Organic Framework, bifunctional catalyst, Hydrothermal method

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Kinetic Study of Hydrogen Oxidation/Evolution Reactions on Nickel in Alkaline Medium

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Abstract

The rate of hydrogen oxidation and evolution reactions (HOR/HER) on nickel (Ni) foil is investigated in 0.1 M and 1 M XOH ($X = K^+$, Na^+ , Li^+) solutions with varying cation concentrations.¹⁻³ The exchange current density is determined from the micropolarization region after correcting the measured current for ohmic drop, back reaction, and mass transport effects.⁴ The activated Ni electrode, which is covered by oxide species, exhibits increased HOR/HER activity. However, the activity in 1 M XOH is lower compared to 0.1 M XOH, suggesting inhibition by either OH^- or X^+ ions. To further elucidate the role of X^+ ions, HOR/HER was studied across a range of cation concentrations. The observed continuous decrease in the kinetic current with increasing cation concentration indicates cation inhibition during HER. This conclusion is further supported by the negative reaction order with respect to the cations in both pH conditions.

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Durable, Efficient, and Cost-Effective Anion Exchange Membrane in an Affordable Alkali Water Electrolyzer for Green Hydrogen Production

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Abstract

In this work, we synthesize a block copolymer using aryl and polycyclic aromatic moiety using an acid-catalyzed^{1,2} polymerization method to prepare a cost-effective anion exchange membrane. The incorporation of polycyclic moiety in the polymer backbone enhances thermal, mechanical, dimensional, and electrochemical properties. The developed membrane had superior ex-situ alkali stability and hydroxide ion conductivity compared to the commercial FAA-3-50 anion exchange membrane. The use of an anion exchange membrane in electrolyzer applications will improve catalyst selectivity while lowering membrane costs.³ As a consequence, the total cost of electrolyzers will be reduced. In dry cathode electrolyzer performance, the obtained current density was three times higher than the commercial FAA-3-50 membrane-based electrolyzer in the same operating condition. The electrolyzer fabricated from the synthesized membrane showed very stable (> 500 h) in 1 M KOH at 60 °C.

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Highly Dispersed Ultrafine Feni-Phosphide Nanoparticles Embedded in Amorphous FeNiO_x for Oxygen Evolution Reaction

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Abstract:

Metal phosphides are considered as highly active electrocatalysts for water splitting. However, they lose their catalytic activity over time via converting to corresponding metal oxides. The situation becomes more complicated when seawater is used instead of de-ionized water as electrolyte. Seawater is abundant on our earth but the presence of Cl⁻ ions compete with the oxygen evolution reaction (OER) and corrodes the electrode fast. Therefore, an acceptable strategy for designing the OER and hydrogen evolution reaction (HER) is necessary to achieve the goal of this objectives. During the OER process of metal phosphides, a layer of metal oxides and phosphate anions are also formed which hinders the access of Cl⁻ to the actual metal phosphide sites and thus prevents the chlorine evolution or OCl⁻ formation in the electrolytes. However, protecting these metal phosphides within second OER active catalysts can further boost the catalytic activity and will also hinder the fast degradation of electrodes during seawater electrolysis. Herein, we report ultrafine FeNi-phosphide (FeNiP_x) nanoparticles embedded in FeNi-oxide (FeNiO_x) nanosheets directly grown on Ni foam for excellent OER electro catalysis. The strong synergistic interactions between the FeNiP_x and S-FeNiO_x are confirmed by spectroscopic methods. The catalyst shows a high current density of 400 mA cm⁻² at an over-potential 380 mV for OER. The excellent durability of catalyst for 200 hours without any significant loss in real seawater electrolyzer makes the catalyst one of the most active and stable anodic electrodes for seawater electrolysis. The FeNiP_x/FeNiO_x/NF was further assessed in a home designed zero-gap flow cell electrolyzer, keeping the Pt mesh at cathode. The cell reaches a tremendous current density of 5 A cm⁻² at supplied voltage of just ~1.7V only.

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Ni/NiO/N Doped Graphene Coated Nickel Foam for Advancing Urea Degradation and Hydrogen Production in Urea-Enriched Wastewater

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Abstract:

Rising global energy demand depletes fossil fuel reserves and contributes to elevated CO₂ levels in the atmosphere. It is imperative to explore and innovate alternative energy technologies to safeguard the global ecosystem. Urea, as a promising hydrogen carrier, holds potential as an alternative energy reservoir for hydrogen-based systems. The electrochemical urea oxidation process (UOR) presents a way to both eliminate urea from wastewater and generate hydrogen simultaneously. In this study, we synthesized a non-noble metal-based catalyst, Ni/NiO/N doped graphene via chemical vapour deposition method and evaluated its electrocatalytic performance for UOR in alkaline urea rich solutions. Cyclic voltammetry (CV) examinations revealed that exhibited the onset potential of 0.32 V (vs Ag/AgCl) and a current density of 100 mA/cm² was achieved at 0.61 V. The incorporation of NiO/N doped graphene mitigated charge transfer resistance, as indicated by Nyquist plots. Additionally, chronoamperometry demonstrated the electrode's stability over time. These findings suggest that modified Nickel foam holds promise as an electrode material for constructing urea electrolyzer, offering a viable solution for the electrochemical treatment of urea-rich wastewater and recovering hydrogen from it.

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Temperature-dependent Investigation of ORR Kinetics on Non-Precious Metal-free Catalysts in Alkaline Media - Doping Effect on Electrocatalysis

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Abstract

Oxygen reduction reaction ORR is investigated on Vulcan XC-72 (C) and a metal-free nitrogen-doped ($\sim \leq 1\%$) carbon (N/C-900) catalysts in 0.1 M KOH [1]. The experiments are conducted in the temperature range of 293–323 K using a rotating ring disk electrode (RRDE) assembly to quantify the product distribution, viz., OH^- and HO_2^- . The measured kinetic current (i_k) is partitioned into i_{k,OH^-} and i_{k,HO_2^-} based on the potential-dependent product distribution (OH^- and HO_2^-) and is used in the estimation of kinetic parameters [2]. The α values are derived from Tafel equation at high overpotentials (η), and the derivative of the change in Gibbs free energy of activation ($\Delta G^\ddagger$) concerning η [3]. The i_k due to the reduction of O_2 to HO_2^- is estimated and used in the Eyring analysis to determine the change in enthalpy of activation ($\Delta H^\ddagger$). It is shown that doping of carbon with nitrogen (even with ≤ 1 wt.%) causes a substantial increase in the number of active sites (almost two-fold) and a reduction in $\Delta H^\ddagger$ at any η . Moreover, $\Delta H^\ddagger$ is a stronger function of η on N/C-900 as compared to that on the carbon surface.

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Surface Mediated Growth of Polyacryloyl Hydrazide Promoted $\text{Co}_3\text{O}_4@\text{NiCu}$ Alloy Nanocuboids for Alkaline Methanol Oxidation Coupled H_2 Production

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Abstract

Advanced alloy-based electrocatalyst development for the alkaline methanol oxidation reaction (MOR) has great potential to produce H_2 and value-added organic compounds, but there are still challenges to overcome. The effectiveness of a catalyst is largely dependent on its size, shape, doping, and morphology. Herein we developed the new one-pot hydrothermal synthesis of $\text{Co}_3\text{O}_4@\text{NiCu}$ alloy nanocuboids on Nickel foam (NF) surface. NF is the source of Ni which controls the shape of nanostructure and PAHz is a capping and reducing agent. Combining the obtained bifunctional electrodes with MOR shows effective green H_2 generation with the valuable selective chemical production of formate. The NF-PAHz- $\text{Co}_3\text{O}_4@\text{NiCu}$ electrode has a high value of j (current density) 0.6 A/cm^2 at $1.54 \text{ V}_{\text{RHE}}$ for MOR and a low overall potential (MOR+HER) of 1.86 V at 0.2 A/cm^2 current density. The electrode exhibits OER activity, attaining a sufficiently stable 0.05 A/cm^2 at $1.61 \text{ V}_{\text{RHE}}$. The DFT simulations reveal that the incorporation of Co-O doping in NiCu alloy effectively enhances catalytic activity and reduces reaction energy barriers for the rate-determining step in MOR and OER studies. There is a potential application for developing other transition metal-based alloy nanostructures for electrocatalytic uses using this adaptable and scalable synthetic method.

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Carbon-Negative eFuel: Advancing Direct Air Capture with Saltwater Electrolysis

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Abstract

In the current study, we explore the potential of saltwater electrolysis (chloralkali) for the synthesis of eFuels (eMethanol). The study explores the use of chlorinated water in carbonate-loop pH-swing “cold capture” of carbon dioxide, and the resulting synergetic integration of the chloralkali process in eFuel syntheses. Doing so eliminates the high energy consumption of calciner and slaker of the benchmarked carbonate-loop thermal-swing method of Direct Air Capture (DAC). It is replaced with a spontaneous chemical process in which chlorine is neutralized in the presence of carbonates. This allows the simultaneous solution of “The Chlorine Problem” of saltwater electrolysis, and a lower overall energy consumption of direct air capture when combined with green hydrogen synthesis. The only limitation on the comparison is that a large amount of carbon dioxide is over-captured when using chloralkali. That is, the ratio of hydrogen generated to carbon dioxide captured is fixed by the stoichiometry of chloralkali and not that of the eFuel. This results in an excess of carbon captured and thus a carbon-negative eFuel. The process captures 300% more CO₂ than is released upon combustion, achieving a 76% carbon capture efficiency and a 79.5% overall process efficiency, representing a significant improvement over benchmark methods.

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Insights of the Efficient Hydrogen Evolution Reaction Performance in Bimetallic Au₄Cu₂ Nanoclusters

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Abstract

The design of efficient electrocatalysts for improving hydrogen evolution reaction (HER) performance using atomically precise metal nanoclusters (NCs) is an emerging area of research. Here, we have studied the HER electrocatalytic performance of monometallic Cu₆, Au₆ NCs, and bimetallic Au₄Cu₂ NCs.^{1, 2} Bimetallic Au₄Cu₂/MoS₂ composite exhibits excellent HER catalytic activity with an overpotential (η_{10}) 155 mV vs reversible hydrogen electrode observed at 10 mA/cm² current density. The improved HER performance in Au₄Cu₂ is due to the increased electrochemically active surface area and the Au₄Cu₂ NCs exhibit better stability than Cu₆ and Au₆ systems and bare MoS₂. This reveals a greater number of active sites for the favorable adsorption of reaction intermediates. Further, from XPS and Raman analysis, the kinetics of HER in Au₄Cu₂/MoS₂ composite were elucidated, attributing the favorable performance due to the better electronic interactions occurring between Au₄Cu₂ NCs and MoS₂ substrate. Theoretical studies reveals that the inherent catalytic enhancement in Au₄Cu₂/MoS₂ is due to favorable H atom adsorption and the smallest ΔG_{H^*} value. The downshift in the d-band of the Au₄Cu₂/MoS₂ composite influences the binding energy of intermediate catalytic species. This new catalyst sheds light on the structure-property relationship for improving electrocatalytic performance at the atomic level.

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Stabilizing Ru Single Atom Catalyst Through Electronic Metal-Support Interaction with NiCo_2O_4 Support for Overall Water Splitting and Urea Electrolysis

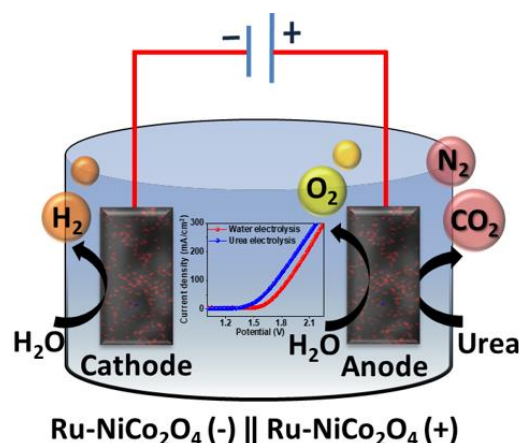
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Abstract

Developing effective bifunctional electrocatalysts in water-splitting becomes crucial in order to avert a massive energy crisis in the near future.¹ Noble metals show an irreplaceable activity toward electrocatalytic water-splitting reactions but their high cost prevent their large-scale application.² Single atom catalyst manifests themselves as a new frontier in heterogeneous catalysis owing to their efficiency of maximum atom utilization.^{3,4} However, their tendency to get aggregate leads to the poor stability, which limits their application.⁵ Herein, we overcome this challenge by stabilising a noble metal single atom catalyst through anchoring it on a metal oxide support, where a strong electronic metal-support interaction prevents their aggregation. Specifically, we have synthesized Ru single atoms anchored on the NiCo_2O_4 support by using the ultra-low amount of Ru. XAS and HAADF-STEM analysis confirms the presence of isolated Ru single atoms on the support. These isolated Ru atoms have a high density of unoccupied orbitals, which is favourable for electrocatalytic activity. The synthesized Ru single atom catalyst on NiCo_2O_4 shows superior activity for overall water splitting with a cell potential of 1.57 V to generate a current density of 10 mA/cm^2 and showing durability of 60 h. Density functional calculation reveals that supported single Ru atoms optimized the binding energies of the intermediate of both HER and OER.



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A Facile Synthesis of Conductive Metal-Organic Frameworks on Electrospun Core-Shell Graphene Nanofiber as Free-Standing Electrodes for Flexible Hybrid Supercapacitors

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Abstract

The development of wearable and flexible energy storage devices depends on freestanding and flexible electrodes. For new-generation supercapacitors, rational modification of graphene is essential to the creation of flexible and freestanding carbon-based electrodes with excellent potential as energy storage facilities. Herein, a novel freestanding/flexible electrode made of porous reduced graphene oxide carbonized nanofiber (rGO/CNF) is constructed via a sequential technique that involves electrospinning and an in situ NiCo-c-MOF growth on it. NiCo-c-MOF@rGO/CNF revealed a specific capacitance of 1820 F g⁻¹ at 1 A g⁻¹, superior rate capability, high cycling stability (92.2 % capacitance retention after 14,000 cycles) with excellent mechanical flexibility because of their high specific surface area, wettability, conductivity, and abundance of active sites. In addition, the flexible asymmetric devices, composed of NiCo-c-MOF@rGO/CNF as the cathode and rGO/CNF as the anode exhibit high energy densities of 52.2 Wh kg⁻¹ and 799.6 Wh kg⁻¹ respectively. These also have good rate capability and long-life cycle stability of 90.6 % after 12000 cycles, indicating their realistic use. This work offers a different approach to high-performance graphene-decorated NF freestanding electrode preparation, and the method can be used with various 2D materials to create effective electrodes for flexible supercapacitors.

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Preventing HER and Unveiling Active Sites on Surface-Modified MXene ($\text{Ti}_3\text{C}_2\text{T}_x$) Supported Metal Hexacyanoferrate to Enhance Nitrogen Reduction Reaction for Ammonia Synthesis

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Abstract

A viable approach to the environmentally friendly and sustainable manufacturing of ammonia is developing an effective, stable, and selective electrocatalysis system for the electrocatalytic N_2 reduction reaction (ENRR)^[1]. Numerous electrocatalysts have been reported, but the significant challenge encountered in this electrochemical synthesis is the selectivity between the NRR and the competing hydrogen evolution process (HER), resulting in poor faradaic efficiency^[2]. Moreover, the real parameters determining the selectivity between the hydrogen evolution reaction (HER) and electrochemical nitrogen reduction reaction (ENRR) remain largely unexplored in this field. Recently, MXene-based catalysts have been found to show remarkable benefits for a variety of catalytic processes, including those involving the evolution of hydrogen and the reduction of oxygen. MXenes however, lack sufficient activity for electrochemical nitrogen reduction because of their surface-terminated inactive functional groups like F and OH, which promote the HER^[3]. Here, we demonstrate the strategy to limit the competing HER and promote NRR with the exploration of possible active sites responsible for N_2 adsorption and activation. In this context, we have synthesized PBA/MXene composite in various weight ratios, where the 2D structure of MXenes provides robust support for PBAs, boosting their mechanical and chemical stability, while the PBA particles, in turn, prevent the restacking of MXene sheets and mask the F and OH functionalities responsible for HER and thus enhance the overall NH_3 yield rate and faradaic efficiency.

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Basal Plane Functionalization of Ti₂C Mxene for Boosted Ammonia Electrosynthesis: Kinetic and Mechanistic Aspects Induced by the Surface Terminated Groups

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Abstract

Altering the edge sites of 2D MXenes for electrochemical N₂ fixation performance has been widely reported, whereas activation of its relatively inert basal planes has been neglected. Herein, we report the modulation of the electrochemical work function (ϕ_{ad}^0) and the potential of zero charge (E_{PZC}) by the activation and the optimization of the basal planes of Ti₂CT_x MXenes (where T_x is the surface terminating functional groups, viz., *F, *O, and *OH) for enhanced electrochemical N₂ reduction reaction (ENRR) to ammonia. Our results show that the fine-tuned composition of the surface terminated functionality alters the local electronic environment which regulates the reaction kinetics. We noted that the relative hydroxyl density (ρ_{ECSA}) normalized with electrochemical active surface area enables higher potential screening for ENRR than hydrogen evolution reaction (HER). The electric field localization modulates the reaction dynamics by stabilizing the transition states and thus lowers the activation energy (ΔE) for ENRR. Moreover, the analysis from hydrodynamic voltammetry, in-situ Raman spectroscopy, and post-electrolysis XPS suggests faster ENRR kinetics which follows associative distal pathway with *OH and F* terminated Ti³⁺ as a dominant ENRR active site over Ti₂CT_x surface.

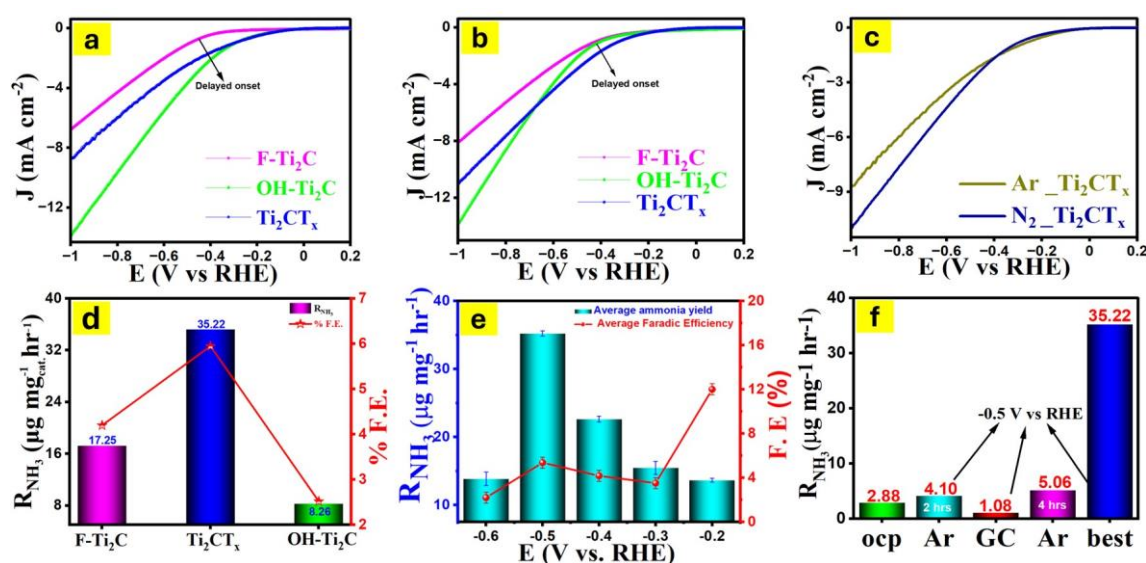


Figure 1: LSV response for MXenes under (a) Ar and (b) N₂ purged at 100 mV s⁻¹ (c) Ar and N₂ purged LSV response for Ti₂CT_x, NH₃ yield rate and % F.E. comparison for (d) different MXenes (e) Ti₂CT_x at various potentials, and (f) background tests under variable conditions in 0.05 M H₂SO₄.

Tailoring the Interfacial Water Structure by Electrolyte Engineering for Selective Electrocatalytic Reduction of Carbon Dioxide

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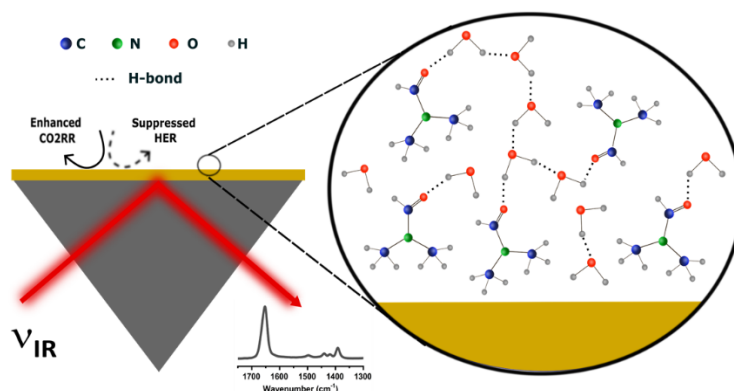
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Abstract

Engineering aqueous electrolytes with low amounts of additives to achieve a tunable CO₂ reduction product is an underexplored territory in electrocatalysis.¹ Here, we show the enhancement of the Faradaic efficiency (FE) of CO₂ reduction to CO on unmodified polycrystalline gold from ~67% to ~94% by the addition of up to 15 mol % of N, N-dimethylformamide (DMF) to an aqueous electrolyte. The role of water structure modification near the electrode-electrolyte interface was studied using in situ surface-enhanced infrared absorption spectroscopy in the attenuated total reflection mode (ATR-SEIRAS).² In addition to the expected detection of the adsorbed CO (CO_{ad}) intermediate present on the Au surface, in both the linearly- and bridged-bonded forms, we observed changes in the structure of interfacial water induced by the addition of DMF. The changes in the water stretching band and the DMF carbonyl band indicate an increase in the strongly hydrogen bonded DMF-water pairs with increasingly negative potential near the interface in the presence of DMF. We hold this interfacial water structure modification by DMF responsible for increasing the CO₂RR FE and decreasing the competing hydrogen evolution reaction (HER). Furthermore, the suppression of the HER is observed in other electrolytes and also when platinum was used as electrode, and hence can be a potential method for increasing the product selectivity of complex electro-catalytic reactions.



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Oxygen Vacancy-Mediated Ethylene Oxidation by Doped Metal Oxide Nanoparticles

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Abstract

Ethylene is a low molecular weight volatile hydrocarbon found indoors and outdoors.¹ Ethylene in the air has been linked to photochemical smog and widespread food spoilage in warehouses. The complete oxidation of ethylene is essential for the sustainable health of humans and the environment. Oxygen vacancies play a significant role as active sites in the thermal catalytic oxidation of ethylene by transition metal oxides.² Ion doping and interphase formation enhance vacancy formation in metal oxides.³ Here C- doped CVD synthesized Co_3O_4 and the resultant material showed better activity towards ethylene oxidation. The catalysts can be applied as automobile exhaust liners, installed in warehouses and indoor air purifiers.

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Organocatalytic Asymmetric Synthesis of α -Arylcyclohexenones from Arylacetones and α,β -Unsaturated Aldehydes

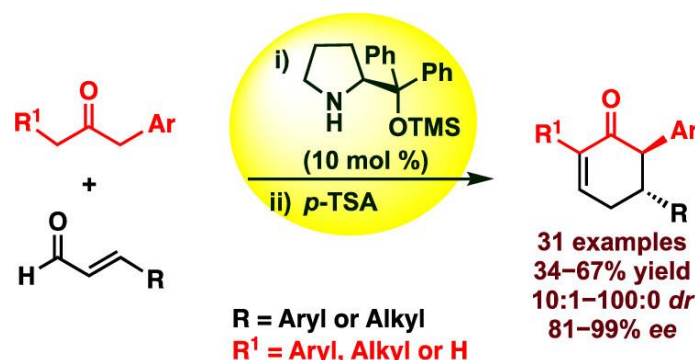
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Abstract

Chiral cyclohexenone is a common structural motif in natural products and pharmaceuticals.¹ Asymmetric synthesis of cyclohexenones via Michael addition followed by aldol condensation (Robinson annulation) is mainly restricted to the reaction between ketones (a ketone and an α,β -unsaturated ketone). In spite of the fact that α -arylcyclohexenones were used as an intermediate for the total synthesis of natural products,² there are very few reports known for the racemic or asymmetric synthesis of α -arylcyclohexenones.³ Here in this a general methodology for the asymmetric synthesis of α -arylcyclohexenones from arylacetones and α,β -unsaturated aldehydes catalyzed by diphenylprolinol silyl ether followed by *p*-TSA-mediated cyclization is developed. A variety of arylacetones and α,β -unsaturated aldehydes were successfully converted to α -arylcyclohexenones in 34–67% yield, 10:1–100:0 *dr*, and 81–99% *ee*. The scalability of this methodology by a gram-scale synthesis and their utility by converting the product to the corresponding epoxide, alcohol, and diol are demonstrated.⁴



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Renormalization of Band-Gap due to Electron-Phonon Coupling in FeBi₄S₇

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Abstract

Using first-principles simulations, we study the band-gap renormalization in one member of transition metal bismuth ternary chalcogenide, FeBi₄S₇^[1], as a function of hydrostatic pressure, focusing on the importance of electron-phonon coupling in such materials in determining the electronic properties. FeBi₄S₇ is a quasi-one-dimensional antiferromagnet that contains chains of edge-sharing iron-sulphide (FeS₆) octahedra. We report on the ground state magnetic structure and the origin of electronic properties in the presence and absence of spin-orbit coupling, which matches well with other reported studies^[2,3,4]. The application of hydrostatic pressure leads to structural transition with a strong reduction in the band-gap. Additionally, the presence of electron-phonon coupling confirms the substantial impact of lattice vibrations on the electronic band structure, leading to bandgap renormalization at different temperatures and pressure. Furthermore, we propose to investigate the role of exciton-polaron coupling in this strongly correlated system by including both Density Functional Theory (DFT) and Bethe-Salpeter Equation (BSE). This coupling could lower the exciton energy, thereby localizing the excitonic-polaron due to the presence of a strong exciton-phonon interaction.

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Large-Area Vacancy Ordered Perovskite Films Development for Photo-Electrocatalytic Hydrogen Generation

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Abstract

Vacancy-ordered double perovskites (VODPs) of A_2BX_6 stoichiometry are potential alternatives to lead containing perovskites of ABX_3 stoichiometry in various applications, especially catalysis, owing to their excellent air and moisture stabilities and better solution processabilities. As in case of other perovskites, their large area synthesis using a facile method remains as a bottleneck. Here we demonstrate the possibilities of their large area synthesis using an electrochemical method, and demonstrate the stability and potential applications of such films in catalysis. A mechanistic insight in to the growth mechanism is provided leading to possibilities of the development of a series of different VODPs, and their efficacy towards photo-electrocatalytic hydrogen generation is demonstrated. Details of the large area synthesis, stability, photocatalytic hydrogen generation etc. will be discussed during the presentation.

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Impact of rGO Variation on Fe₂O₃ Anode Performance in Li-Ion Batteries

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Abstract

The advancement of sustainable anode materials with high capacity, rate capability, and cycling stability is crucial for the development of high-performance Li-ion batteries (LIBs). While graphite is widely used due to its favourable electrochemical properties, its theoretical capacity of 372 mAhg⁻¹ limits its applicability in demanding applications. In contrast, Fe₂O₃ presents a significantly higher theoretical capacity (~1007 mAhg⁻¹) and thus represents a promising alternative. Nevertheless, Fe₂O₃ experiences considerable volume expansion during lithiation and delithiation, which adversely affects its electrochemical stability and cycling performance. To mitigate these issues, Fe₂O₃/carbon composites have been explored to enhance electrical conductivity and prevent nanoparticle aggregation, thereby improving electrochemical performance. In this study, α -Fe₂O₃ nanoparticles were synthesized on reduced graphene oxide (rGO) using a solvothermal process to improve the electrical conductivity of Fe₂O₃ and leverage the porous structure of rGO to accommodate volume changes during Li-ion cycling. The rGO content was systematically varied to identify the optimal amount of GO for effective composite fabrication. The resulting materials were characterized by X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), Fourier-transform infrared spectroscopy (FTIR), and Raman spectroscopy. The impact of varying rGO contents on the anode material's performance was assessed through cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and galvanostatic charge-discharge (GCD) tests.

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Shorter Ionic Pathed Solid Electrolyte Materials for Next-Generation Batteries

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Abstract

Solid-state batteries are a promising technology, offering higher energy density, improved flexibility, and enhanced safety¹. However, they are challenged by issues such as high interfacial resistance, lattice mismatch, and low ionic conductivity^{2,3}. In this study, we developed Ga-Fe doped $\text{Li}_{6.25}(\text{Ga}_{0.125}\text{Fe}_{0.125})\text{La}_3\text{Zr}_2\text{O}_{12}$ with a panicle morphology, later converted into a flexible substrate with an ionic conductivity of $2.96 \times 10^{-3} \text{ S/cm}$, surpassing that of conventional 3D LLZO materials⁴. The panicle structure plays a crucial role in shortening the ionic transport path and reducing lattice mismatch between the electrode and electrolyte. Its soft-network design also lowers interfacial resistance at the electrode/electrolyte interface, enhancing ion movement through the electrolyte. Additionally, this material exhibits a wide electrochemical stability window and compatibility with low-temperature operations, while maintaining excellent properties. This improvement leads to better battery performance, extended lifespan, faster charging times, and higher energy densities—critical advancements for next-generation energy storage technologies. This breakthrough marks a significant step toward safer, more durable solid-state batteries.

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2D $\text{CaCoO}_2\text{--CoO}_2$ Nanosheets: Advancing Supercapacitor Performance through Exfoliation and Pseudocapacitive Charge Storage

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Abstract

Layered materials have attracted considerable attention due to their unique properties, which make them highly suitable for applications in energy storage, catalysis, and sensing. Among them, two-dimensional (2D) systems offer enhanced performance owing to their large surface areas and exceptional electrochemical properties. This study focuses on the nanostructuring of $\text{Ca}_3\text{Co}_4\text{O}_9$ (CCO), a well-known oxide-based misfit-layered compound (MLC), into 2D nanosheets of $\text{CaCoO}_2\text{--CoO}_2$ (CCONS) for use as supercapacitor electrodes. The exfoliated CCONS nanosheets exhibited significantly improved surface area and accessibility to active sites, facilitating charge storage through pseudocapacitive mechanisms. Electrochemical testing shown specific capacitances of 242 F/g in 1 M LiOH and 247 F/g in 3 M KOH at 0.3 A/g. The nanosheets retained 77% and 65% of their capacitance after 5000 and 2200 cycles in LiOH and KOH, respectively. Remarkably, CCONS demonstrated a 17-fold increase in capacitance in LiOH and a 15-fold increase in KOH compared to bulk CCO. This work represents the first report of using nanostructured calcium cobalt oxides as supercapacitor electrodes, highlighting their potential for enhanced energy storage applications. Electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV), and galvanostatic charge-discharge (GCD) measurements were employed to investigate the charge storage mechanisms in detail.

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“Acyl Silane Additives” Enabled Stable Cycling Lithium Metal Batteries

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Abstract

The high theoretical capacity of lithium (Li) metal i.e., 3860 mAh g⁻¹ and its low electrochemical potential i.e., -3.04 V vs. the standard hydrogen electrode (SHE) makes it the most appealing anode material for high energy density Li batteries. LiPF₆ salt dissolved in organic carbonate-based solvents is one of the most widely used electrolytes in Li batteries.¹ However, its sensitivity towards moisture/air leads to the decomposition and release of toxic and corrosive hydrogen fluoride (HF) gas. The evolved HF gas results in transition metal dissolution in the cathode side. Ultimately, the decomposition of electrolytes, the formation of a thick SEI layer on the anode, and the destruction of the cathode cause severe capacity loss. Electrolyte formulation using additives is one of the means employed to mitigate Li dendrite formation and scavenging HF.² Numerous organosilicon-based additives have been reported, capable of improving the battery performance by acting as acid scavengers and forming a stable uniform anode passivation layer to impede nonuniform lithium dendrite growth.³ In this research, a new-type of electrolyte additive-di-methyl amino di-tert-butyl adamantoyl silane (bis(di-tert-butyl methyl silyl ketone) [(RR'Si)₂CO], where R is (tBu)₂ and R' is CH₃) is introduced to improve the electrochemical performance of Ni-Rich/Li metal batteries containing 1 M LiPF₆ and EC:EMC (3:7) as the electrolyte. The cell with the presence of additive demonstrated remarkably better performance than the base one.

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Engineering Cobalt Sulfide Electrocatalyst Through Citric Acid Directed Sulfidation for Overall Water Splitting

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Abstract

Cobalt sulfide based electrocatalysts are gaining interest due to their potential for efficient and economical total water splitting¹, which is an essential step in the production of hydrogen and renewable energy². The present study investigates the role of citric acid in sulfidation process that impacts the catalytic performance in hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). Citric acid acts as a chelating agent, co-ordinated with cobalt metal ions to regulate their release, thereby promoting the formation of well-defined CoS nanostructures with increased active sites and surface area³. Tuning the concentration of citric acid influences in adjusting the material's shape, surface characteristics, and catalytic activity during the sulfidation of CoS. All the developed CoS electrocatalysts were tested for water splitting reaction in 0.1 M KOH. The electrocatalyst with Co: citric acid (1:8) demonstrates a small tafel slope of 40 mV dec⁻¹ with a lower overpotential potential of -0.18 V versus RHE for HER whereas for OER a tafel slope of 109 mV dec⁻¹ with an overpotential of 1.52 V versus RHE to generate 10 mA cm⁻² current density. This work paves avenues to construct commercially viable, low cost, high performing cobalt sulphide electrocatalysts for the production of hydrogen and oxygen.

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Fe-MIL-101-NH₂ modified by ovan-Schiff-Base-Ni: A Novel Electrochemical Sensor for Environmental Hazardous Phenolic Compound

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Abstract

The present study is aimed at the fabrication of an electrochemical sensor by post-synthetic modification of Fe-MIL-101-NH₂ with o-vanillin followed by successful anchoring of the Nickel by the addition of Nickel Sulphate for the determination of 4-AP. MOF based on Iron had been modified by the reaction of o-vanillin (ovan) with the amino groups to form ovan-imine that acts as a ligand of various metals M (where M = Ni). X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), Energy dispersive X-ray analysis (EDX), Thermogravimetric analysis (TGA), and Scanning electron microscopy (SEM) analysis were used to characterize Fe-MOF. Under ideal conditions, the electrochemical sensor showed a linear range over a concentration range from 0.5-400 μ M with a limit of detection (LOD) of 0.12 μ M. The sensor fabricated through the surface modification of Fe-MIL-101-NH₂ has enhanced stability and is cost-effective owing to the presence of earth-abundant metals. The sensor has unique features like reusability, sensitivity, selectivity for 4-AP, and minimum organic and inorganic species interference. The synergistic effect of Fe-MIL-101-NH₂, Schiff base, and Ni leads to improved electronic properties of the fabricated sensor such as lower band gap energy, charge transfer resistance, and improved conductivity which further results in enhanced redox behavior of 4-AP. Excellent electrochemical behavior implies real-world applications for the sensor which will be presented.

Battery Materials Particle Cracking Detection by Acoustic Emission

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Abstract

Decarbonization and electrification of automobile industry opened market for battery manufactures in large scale¹. It is essential to qualify the battery cells in the manufacturing stage non-destructively. One of the best non-destructive techniques to diagnose the lithium-ion battery (LiB) is Acoustic Emission (AE) technique, which involves passive observation of elastic waves generated during minute changes in battery². AE technique involves capturing the wave form using suitable AE sensor placed on the surface of the battery, amplifying the signals using preamplifier, Fast Fourier Transform (FFT) analysis³ to get AE parameters and further data processing to diagnose the failure mode of the battery. Active material (AM) particle cracking is one of the familiar failure phenomena in NMC based cathode materials in LiB. In our study, we aimed to establish the relationship between particle cracking and operating conditions such as C-rate, Upper cutoff voltage, Temperature using AE technique. This study began with AE frequency identification to which the response is substantial and later extended to the parametric study to identify the impact of operating conditions. It is concluded that AE studies explain AM particle cracking efficiently for LiB diagnosis.

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Green Synthesis of a Magnesium Single-Atom Catalyst from *Spinacia Oleracea* Chlorophyll Extracts for Sustainable Electrocatalytic Nitrate Reduction to Ammonia

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Abstract

Herein, we report a practically viable magnesium SAC (MgN_xC) for the promising reduction of nitrate to ammonia. The catalyst was prepared using green leaf extracts of *Spinacia oleracea* via simple one-step pyrolysis. We optimized their synthesis temperature to scrutinize the effect of SAC formation and their variation on the catalysis efficacy. The $\text{MgN}_x\text{C650}$ catalyst, anchored on a defective graphitic matrix, exhibits the best-optimized potential of -0.58 V vs. RHE, a faradaic efficiency of $81.5 \pm 2.9\%$ and a yield rate of $392.5 \pm 41.2\text{ }\mu\text{mol h}^{-1}\text{ mg}^{-1}_{\text{cat}}$ with excellent repeatability. DFT is employed to optimize the most stable reactive site and various reaction pathways for favorable nitrate reduction reaction with probable reaction intermediates were explored. Collectively, our work demonstrates a simple, cost-effective, and convenient way to synthesize SACs.

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Site-Specific Substitution and Concomitant Modulation in Properties of Atomically Precise Carboranethiol-Protected Ag₁₇, AuAg₁₆, Ag₁₃Cu₄ and AuAg₁₂Cu₄ Clusters

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Abstract

This study explores the photophysical properties of atomically precise M₁₇ nanoclusters (NCs) with an M@M₁₂@M₄ structure, protected by ortho-carborane-1-thiol (o₁-CBT). The parent cluster, [Ag₁₇(o₁-CBT)₁₂]³⁻ (**Ag**₁₇), consists of a central icosahedral Ag₁₃ core and a tetrahedral Ag₄ shell. Site-specific alloying of Au and Cu atoms produced bimetallic and trimetallic NCs: **AuAg**₁₆, **Ag**₁₃**Cu**₄, and **AuAg**₁₂**Cu**₄. Structural analysis using mass spectrometry and single-crystal X-ray diffraction confirmed their compositions, with theoretical calculations validating Au's preference for the core and Cu for the outer shell. Alloying enhanced structural stability and broadened the HOMO-LUMO gap, increasing from 2.09 eV for **Ag**₁₇ to 2.28 eV for **AuAg**₁₂**Cu**₄. **Ag**₁₇ exhibited fluorescence, while Au incorporation stabilized excited states, and Cu substitution significantly extended excited-state decay lifetimes, resulting in phosphorescence. Ultrafast transient absorption studies revealed structure-specific excited-state relaxation dynamics.

This work demonstrates the first carborane-thiol-protected trimetallic NC, showcasing tunable luminescence and decay lifetimes through precise metal placement. The unique combination of bright luminescence, structural porosity, and stability positions these NCs as promising candidates for applications in catalysis, sensing, and molecular trapping. These findings highlight the potential of systematic heteroatom incorporation in designing advanced atomically precise photoemitters.

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Preferential Production of CH₃OH from both CO₂ and CO by an Mn(I)- Based Molecular Catalyst-Anchored Electrolyzer Assembly

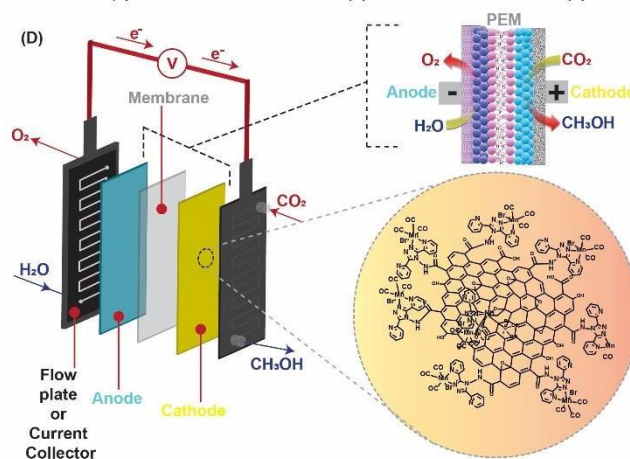
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Abstract

The worldwide carbon dioxide emissions have doubled over the last three decades and are expected to quadruple by 2040 based on current rates of fossil fuel utilization.¹ Therefore, the intermittent nature of renewable energy production and the necessity to curtail CO₂ emissions must be effectively and wisely managed by utilizing CO₂ as an energy carrier.² Among the various strategies, the electrochemical reduction of CO₂ to value-added chemicals offers a promising solution.³ This process not only reduces atmospheric CO₂ but also converts it into useful products such as methanol (CH₃OH), formic acid (HCOOH), and carbon monoxide (CO), which can be utilized as fuels, chemical feedstocks, and industrial precursors. In this study demonstrates the potential of a Mn complex containing NH₂-functionalized ligand scaffold anchored on graphene oxide (**Mn-adpt@GO**) for efficient electrochemical reduction of CO₂ to CH₃OH in aqueous media. The reduction of CO₂ to methanol was observed to proceed via a CO or CO intermediate, with methanol formation increasing up to twofold when exposed to a mixture of CO and CO₂ gas. Using a flow electrolyzer, the **Mn-adpt@GO** catalyst achieved a current density of 1 A/cm² for CO₂RR and a threefold increase in faradaic efficiency compared to an H-cell setup. Stability tests confirmed the robustness of the catalyst, maintaining structural integrity and catalytic activity over extended periods.



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Perovskite Solar Cells: Addressing Degradation Mechanisms and Scaling Up Commercialization through Innovative Materials and Manufacturing

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Abstract

Perovskite solar cells (PSCs) have emerged as a transformative technology in photovoltaics, boasting efficiencies of up to 30%.¹ Key advantages include low fabrication costs and superior tunability compared to traditional silicon-based solar cells. Our research focuses on developing environmentally friendly, lead-free PSCs and high-efficiency multi-junction cells to enhance efficiency, lifetime, and commercial viability.² We investigated degradation mechanisms in both perovskite materials and surrounding device layers to improve cell durability, a critical factor for commercialization.^{3,4} The primary challenge lies in stability, as PSCs are susceptible to moisture due to inherently weak bonds in the perovskite structure.⁴ To address this, we explored: a) Surface treatments to reduce reactivity b) Alternative perovskite materials and formulations c) Innovative surrounding device layers and electrical contacts d) Advanced encapsulation materials e) Fabrication and operation techniques to mitigate degradation Our synthesis route employs solution-based manufacturing, the most cost-effective and widely used industrial method. This research aims to accelerate the commercialization of perovskite solar technologies, reduce manufacturing costs, and optimize the utilization of solar energy.

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Biochar Derived from Temple Floral Waste: An Innovative Approach for Dye Removal from Synthetic Wastewater

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Abstract

During the religious rituals in temples and other places for worship floral offerings are performed due to which a large amount of waste is generated. The floral waste are commonly discarded into open lands and water bodies thereby affecting the soil and water quality of the nearby environment. This study investigates the potential of converting chrysanthemum and marigold floral waste into biochar through slow pyrolysis, offering a sustainable solution for dye removal from wastewater and promoting a circular economy. Biochar prepared at three distinct temperatures were characterized using TGA, FTIR, SEM, BET, XRD and Raman spectroscopy. Batch adsorption studies were carried for the removal of dyes using the biochars as bioabsorbents from aqueous solutions. The results demonstrate that converting floral waste into biochar provides an effective and environmentally friendly method for managing waste and removal of dye from wastewater, contributing to a closed-loop system.

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A Smart and Sustainable Pathway for Abatement of Single and Binary Mixtures of Dyes through Magnetically Retrievable $\text{Ca}_4\text{Fe}_9\text{O}_{17}$ Anchored on Biochar Matrix

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Abstract

In this work, the author developed $\text{Ca}_4\text{Fe}_9\text{O}_{17}$ /biochar (CFB) via a green method through a facile co-precipitation procedure involving eggshells as calcium precursor and investigating its performance in single as well as binary solution of methylene blue (MB) and rhodamine B (RhB). The degradation efficacy of MB and RhB dyes was achieved at 99.2% and 98.6%, respectively, in a single solution, whereas 99.4% and 99.2%, respectively, in a binary solution within 36 min. Additionally, an iron cluster was formed during the degradation process of MB dye. The degradation of organic contaminants and generation of iron clusters from the degraded dye products were both expedited by the remarkable extension effect of the $\text{Ca}_4\text{Fe}_9\text{O}_{17}$ in the CFB nanocomposites. The three processes were achieved using CFB nanocomposite: (1) the advanced oxidation process; (2) degradation of MB and RhB dye in single as well as binary solution with enhanced efficiency, (3) the production of the iron cluster from degraded products. Thus, these three steps constitute a smart and sustainable way that leads to an effective effluent water treatment system and the generation of iron clusters preventing secondary pollution.

Biopolymer Nanoparticles as Performance Enhancers of Thin Packaging Films

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Abstract

Single use synthetic plastics and waxes extensively used in food packaging started posing alarming threat to the whole eco system especially in the form of microplastics. This can be subjugated with the utilization of biopolymers for single use food packaging films and coatings. Pectin is a abundantly available low cost biopolymer which have favorable characteristics to be used as matrix of packaging film. This research investigates the importance of pectin source on film properties and examines the impact of cellulose nanoparticles in enhancing mechanical and barrier properties of pectin films. Statistical Design of Experiments (DoE) was used for optimizing the process parameters and film composition.

Pectin was systematically extracted from various fruit peels with an yield of $60\pm 5\%$. Thermal analysis confirmed the excellent thermal stability of extracted pectin than commercial pectin. Cellulose nanoparticles (CNP) were synthesized via acid hydrolysis with an yield of $75\pm 2\%$.

The sweet lime pectin films exhibited better moisture barrier properties and mechanical stability than commercial pectin. Further, the extracted pectin films were water-insoluble for over two hours, while commercial pectin films dissolved within 20 minutes. Composite thin films were developed by incorporating CNP, gluten and vegetable oil into pectin. The films were 79 ± 2 microns thick and transparent. The improvement in moisture barrier and mechanical strength ($50\pm 3\%$ elongation at break) of the films was evident with the addition of nanoparticles. Gluten and oil concentration observed to be also critical for transparency and mechanical properties. All films degraded within 2 days in soil. The coating of pectin composite formulation extended the shelf life of capsicum for 15 days compared to uncoated.

In conclusion, biopolymer-based films, with enhanced mechanical and barrier properties, offer a viable alternative to plastic packaging, to extend the shelf life of food products.

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Value-addition of Essential Oils/ Aroma Chemicals through Catalytic Hydrogenation

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Abstract

Tetrahydrolinalool is a key ingredient in fragrance creations ranged from flowers over fruits to wood or citrus note possessed 0.02 µg/l threshold in air. In the present communication, we have shown catalytic hydrogenation of acyclic diene alcohol to dihydrolinalool and tetrahydrolinalool using a newly synthesized catalyst combination of 1%Ni-4%Pd/BC and 2%Ni-8%Pd/AC Nickel/Paladium. The activated carbon (AC) and biochar (BC) were the base materials in prepared catalysts. The catalyst for the synthesis of dihydrolinalool were prepared using a hydrothermal process, and the - BC was obtained from industrial waste biomass of menthol mint (pitch) whereas tetrahydrolinalool synthesis was based on commercial grade AC. The catalysts characterization was carried out using XRD, FT-IR, SEM-EDAX, XPS, TEM, and TGA, to determine the weight percentages of Ni and Pd incorporated into the carbon. The results showed that both 1%Ni-4%Pd/BC and 2%Ni-8%Pd/AC catalysts exhibited high catalytic activity for the hydrogenation of linalool to 6,7-dihydrolinalool and tetrahydrolinalool with high selectivity. Furthermore, the optimized reaction conditions have successfully implemented on linalool rich *Ocimum basilicum* var. *CIM-Shishir* essential oils. Under the validated experimental conditions such as temperature pressure, and a reaction time, etc., the substrate conversion into dihydrolinalool and tetrahydrolinalool (selectivity of 82.5% and 91.6%) were obtained.

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Catalytic Upgradation of Lactic Acid to Ethyl Lactate using Heterogenized Heteropolyacids

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Abstract

To understand how the supports interact with the acid catalyst and enhance its activity, an esterification reaction is performed using a lactic acid to ethanol ratio of 1:5 with three different heteropoly acids (HPAs) at 373 K for two hours in a monowave batch reactor to obtain ethyl lactate. The experiment is repeated thrice to ensure reproducibility of the data. TiO₂ support is heterogenized onto HPAs to form a composite using a protocol described in the literature¹. Various characterization techniques, including XRD, BET, TEM-EDX, and FTIR, are employed to analyse the composite's characteristics and properties. XRD confirms that the material is crystalline, while TEM-EDX and FTIR further validate the loading of HPAs onto TiO₂. On the other hand, BET analysis reveals a decrease in the surface area (SA) of the composite compared to bare TiO₂, though it remains much higher than that of the HPAs. Without any catalyst, the conversion was very low at 18%. In the presence of TiO₂ (SA = 120 m²/g), the conversion increased to 55%. In the presence of the composite (SA = 83 m²/g), the conversion further increased to 75%. This suggests that the reaction is independent on changes in surface area.

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Iron Single-Atom Catalyzed N-Alkylation of Amines with Alcohols via Borrowing Hydrogen Strategy

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Abstract

Non-noble? No problem! The borrowing hydrogen protocol is recognized for its one-pot synthesis of various chemicals and intermediates, with economic and environmental benefits. In this research work, we synthesized N-doped graphene supported Fe-single atoms ($\text{Fe}_{\text{SA}}@\text{N-G}$) using a solution-chemistry ion adsorption strategy. The comprehensive characterization of the synthesized catalyst reveals that the HAADF-STEM and EXAFS analyses provide confirmation of the coordination of isolated Fe atoms with four nitrogens at $\text{Fe}_1\text{-N}_4$ site in $\text{Fe}_{\text{SA}}@\text{N-G}$. The $\text{Fe}_{\text{SA}}@\text{N-G}$ catalyst exhibited remarkable performance in solvent-free conditions for the N-alkylation of amine with alcohol, achieving a high TOF-413.1 h^{-1} . Further, $\text{Fe}_{\text{SA}}@\text{N-G}$ and a suitable base achieved excellent conversion and selectivity more than 50 N-alkylated products from aliphatic and aromatic amines with aliphatic and aromatic alcohol as well as alcohols with the pharmaceutically important molecules under microwave irradiation. DFT study confirmed the mechanistic action of N-alkylation of amines with alcohol, indicating that Fe-H hydride transfer occurs in the $\text{Fe}_1(\text{III})\text{-N}_4$ active site. In addition, $\text{Fe}_{\text{SA}}@\text{N-G}$ exhibits exceptional stability and recyclability, with no discernible decrease in activity even after 5 runs and suitable for N-alkylation reaction at gram scale reaction. The utilization of Fe active site catalysts can prove beneficial in sustainable organic transformations that involve hydrogen transfer.

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Tuning Acidic Characteristics in Amorphous Aluminosilicates Through Defects

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Abstract

Crystalline zeolites are known for their substantial acidity but are limited by microporosity, whereas mesoporous amorphous aluminosilicates offer better porosity but lack comparable acidity.¹⁻³ This study explores the potential of using defects to enhance the acidity of acidic amorphous aluminosilicates (AAS).⁴ We introduced oxygen vacancy sites to create defected acidic aluminosilicates (D-AAS).⁵ ¹H, ²⁷Al and ¹⁷O solid-state nuclear magnetic resonance (ssNMR) spectroscopy showed that these defects cause localized structural changes around acidic sites, thereby modifying their acidity. X-ray photoelectron spectroscopy (XPS) and Fourier transform infrared spectroscopy (FTIR) confirmed that oxygen vacancies alter the chemical environment of Brønsted acidic sites, enhancing overall acidity. Additionally, oxygen storage capacity and ammonia temperature-programmed desorption studies revealed a correlation between defect site concentration and overall catalyst acidity. The impact of defect creation on AAS acidity and catalytic performance was demonstrated through four acid-catalyzed reactions: styrene oxide ring opening, vesidryl synthesis, Friedel-Crafts alkylation, and jasminaldehyde synthesis. The induced defects were found to play a crucial role in activating reactants, thus enhancing the catalytic process. These findings were supported by *in-situ* FTIR studies, which provided insights into the molecular-level reaction mechanisms and the role of defects in reactant activation. This work highlights defect manipulation as a promising strategy to fine-tune the acidity of amorphous aluminosilicates, effectively bridging the gap in porosity and acidity between mesoporous amorphous aluminosilicates and crystalline zeolites.⁵

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Diffusion-controlled Catalysis using Metal-Organic Framework Thin Film

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Abstract

Crystalline nanoporous materials are highly efficient as heterogeneous catalysts. However, the turnover frequency and product selectivity are often underestimated due to significant diffusion limitations of reactants accessing the catalytic sites. To enhance both turnover frequency and selectivity, it is essential to optimize the diffusion length of the reactants. This study presents a method that optimizes reactant diffusion by utilizing a thin film of a porous metal-organic framework (MOF) catalyst¹ within a cross-flow microfluidic reactor. By programming the diffusion and manipulating reactant residence time at the active sites, we demonstrate substantial improvements in catalytic performance, achieving over a 1000-fold increase in turnover frequency and a 2-fold enhancement in geometric selectivity compared to conventional bulk catalysts². The diffusion-programmed strategy represents a significant advancement in the design and application of porous catalysts in organic reactions.

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Skeletal Editing of Pyrimidine into N–N-Bridged Bistriazole via Pyrazole for Applications in Energetic Materials

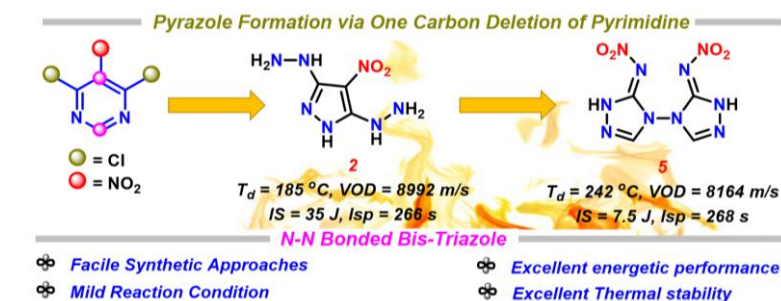
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Abstract

Recent research in energetic materials has focused on developing new compounds that offer enhanced energetic performance while reducing sensitivity to heat, shock, impact, and friction. One promising strategy is the incorporation of nitrogen-rich azoles, which are easy to synthesize and provide balanced performance. In this study, we synthesized several compounds, including 3,5-dihydrazinyl-4-nitro-1H-pyrazole (**2**), 9-nitro-1H-pyrazolo[3,2-c:5,1-c']bis([1,2,4]triazole)-3,6-diamine (**3**), N–N bonded N,N'-([4,4'-bi(1,2,4-triazole)]-3,3'-diyl)dinitramide (**5**), and its stable nitrogen-rich energetic salts, using one or two-step processes with high yields from the inexpensive starting material 4,6-dichloro-5-nitropyrimidine (**1**). Characterization of these compounds was performed using NMR, IR, DSC, and elemental analysis (EA), and their structures were confirmed by single crystal X-ray diffraction studies. Notably, most of the compounds demonstrated excellent thermal stability (ranging from 221 to 250 °C) compared to RDX (210 °C) and achieved detonation velocities between 8992 to 9069 m/s, surpassing RDX (8878 m/s) and approaching HMX (9221 m/s). Additionally, these compounds exhibited low sensitivity to impact (10 to 35 J) and friction (360 N). The novelty, ease of synthesis, and superior energetic performance of these molecules indicate their potential use as secondary explosives in both defence and civilian applications.



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A BaTiO₃/CuO Nanocomposite for Piezoelectrically-Triggered Degradation of Dye, Antibiotic and Bacterial Disinfection

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Abstract

In this study, we introduce BaTiO₃/CuO nanocomposite to enhance piezocatalytic efficiency for environmental remediation. Conventional piezoelectric materials like pure BaTiO₃ nanoparticles face limitations due to the rapid recombination of charge carriers. To address this, BaTiO₃ nanoparticles were wrapped with CuO nanosheets, comprehensively characterized employing Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), Energy dispersive spectroscopy (EDS), X-ray Diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). The nanocomposite demonstrated significant potential in degrading a cationic dye, Rhodamine B (RhB) when exposed to ultrasonication. The degradation percentage for RhB was 3.8 times better in the nanocomposite against BaTiO₃. It also effectively broke down Ofloxacin, a pharmaceutical pollutant, utilizing piezo-activation of peroxydisulphate (PDS). Additionally, the nanocomposite achieved effective piezocatalytic elimination of *Escherichia coli* bacteria within 120 minutes of ultrasonication. The improved degradation performance is credited to the synergistic interplay between the nanocomposite and the piezoelectric field generated by vibration, promoting the separation of charge carriers. Importantly, the synthesized nanocomposite exhibited robust stability over five successive degradation cycles. These findings provide valuable insights into advancing piezocatalytic materials for wastewater treatment applications.

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Halfa Grass Assembled Double-Layered Hydrogel Evaporator for Sunlight-Driven Steam Generation and Selective Uranium Extraction

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Abstract

Fresh drinking water and energy are crucial for the human society to live in a sustainable way, and both of these could be attained from the seawater. Herein, we designed a double-layered hydrogel evaporator (PCG@FCG) by using calcined carbon fiber derived from halfa grass (*Desmostachya bipinnata*) as a light absorbing photothermal material. The bottom hydrophilic layer composed of chitosan (CS), carboxy methyl cellulose (CMC), and amidoxime-modified chitosan (AOC), which helps in water transport to the upper surface of evaporator. The amidoxime modified chitosan helps in selective binding and recovery of uranium from the seawater. Such a judiciously designed PCG@FCG evaporator shows light absorbance of 96%, stable evaporation rate of $2.0 \text{ kg m}^{-2} \text{ h}^{-1}$, having an outstanding selective uranium recovery of 325 mg g^{-1} under one sun irradiation. These outcomes result from the inherent structural porosity, enhanced evaporation rate, and selectively designed uranium binding sites. In addition, excellent salt-mitigating ability to promote uninterrupted evaporation, ability to purify the organic-contaminated wastewater/seawater endow the PCG@FCG evaporator with efficient seawater desalination ability and selective adsorption of uranium from the seawater. Overall, this innovatively designed floating evaporator offers a sustainable approach to utilize the lavish resources in the seawater.

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Nitrogen Shifts Gears for NiOOH Formation in Carbon Support for Efficient Methanol Oxidation Reaction

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Abstract

Hydrogen is considered a green fuel for future generations with a zero-carbon emission strategy. Electrochemical water splitting is a promising method for green H₂ generation. However, its massive production is limited by the use of costly noble metals-based catalysts and sluggish four-electron oxygen evolution reaction at the anode. Methanol upgrading reduces the anodic potential, increasing the H₂ production rate while forming innocuous formate as a by-product. Herein, we have synthesized low-cost nickel-based nitrogen-doped carbon material using high-temperature pyrolysis for methanol oxidation reaction. Nitrogen doping plays a vital role in regulating the size of the nickel nanoparticles and also influences their electrocatalytic behavior. It facilitates the formation of essential redox electroactive NiOOH species at a much lower potential. The anodic potential gap decreased by 210 mV after introducing methanol in the electrolyte. The high electrochemical methanol oxidation activity with ultralow loading of nickel is evident from various electrochemical investigations that reflect the role of nitrogen in ensuring better charge transfer in the nickel nanoparticles. Further, to mimic the operating condition of an alkaline electrolyzer, temperature-based measurements are vital, and temperature-based studies reveal that the potential gap between OER and MOR decreases.

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Sillen–Aurivillius Perovskite Oxybromide $\text{Sr}_2\text{Bi}_3\text{Nb}_2\text{O}_{11}\text{Br}$ as a Fatigue-Free Piezocatalyst with Ultrahigh Hydrogen Evolution Rate

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Abstract

Piezocatalysis for noise harvesting and sustainable hydrogen production is an emerging approach to converting mechanical energy into chemical energy.¹ Therein, ultrasonic noise exerts gigapascal pressure on piezoactive² materials to develop surface-positive and surface-negative charges capable of redox reactions on the opposite facets of its crystal. The advantages include the non-requirement of conducting materials (as in electrocatalysis), band-alignment conditions (as in photocatalysis), and noble metal cocatalysts, leading to a diverse set of highly stable, insulating materials as potential catalysts. We have investigated the polar, double-layered Sillen–Aurivillius^{3,4} perovskite oxyhalide, $\text{Sr}_2\text{Bi}_3\text{Nb}_2\text{O}_{11}\text{Br}$, as a highly efficient and fatigue-resistant piezocatalysts for pure and seawater splitting. These flux-synthesized^{1,5}, single-crystalline, [100] faceted catalyst nanoplates exhibited a very high piezoelectric coefficient and hydrogen production rates of 5.3, 4.1, and 3.5 mmol/g/h in pure, simulated, and real sea waters, surpassing the existing piezocatalysts. A remarkable advancement is the exceptional long-term stability of $\text{Sr}_2\text{Bi}_3\text{Nb}_2\text{O}_{11}\text{Br}$, retaining the catalytic activity for over 150 hours of continuous use, originating from a space-charge neutralization mechanism, while most conventional catalysts experience degradation typically after 10–15 hours. The findings position $\text{Sr}_2\text{Bi}_3\text{Nb}_2\text{O}_{11}\text{Br}$ as a highly promising candidate for the development of durable and efficient piezocatalytic systems for sustainable hydrogen production.

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Mechanistic Insights into the Superior Catalysis by SrTiO₃: Unveiling the oxygen vacancies elevated Piezo-Fenton Synergism

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Abstract

The effectiveness of piezo catalysis relies on generating electrical charges under mechanical stress, which is a trait of non-centrosymmetric crystals. In contrast, centrosymmetric materials like SrTiO₃ lack this property due to their symmetrical structure, which results in significantly lower catalytic activity, posing a challenge in harnessing such materials for piezocatalysis. In this study, we investigated the enhanced catalytic activity of SrTiO₃ (STO) for the degradation of methylene blue (MB) dye by combining the piezocatalytic process with the Fenton reaction. When subjected to ultrasonication, 0.2 g of STO alone degraded only 44% of a 10 ppm MB solution within 4 hours. However, in the presence of 5 ppm Fe²⁺ ions, the same amount of STO demonstrated an enhanced degradation efficiency, achieving 85% degradation under the same conditions. To optimize this process, comprehensive parametric studies were conducted, evaluating factors such as catalyst dosage, Fe²⁺ concentration, and dye concentration. Further investigation into the mechanism behind this improved performance was conducted using reactive oxygen species (ROS) estimation and X-ray photoelectron spectroscopy (XPS) analysis. The presence of Fe²⁺ in the aqueous medium was found to increase the ROS count, primarily due to a continuous redox cycle between Fe²⁺ and the H₂O₂ generated during the process. Additionally, the degradation kinetics were significantly influenced by the extent of oxygen vacancies on the STO surface, underscoring their crucial role in facilitating redox reactions. These findings demonstrate the potential of this synergistic approach to effectively harness the piezocatalytic activity of centrosymmetric materials for environmental remediation.

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Hydrodeoxygenation of Biomass-Derived Cyclic Esters to Alkanes using Ir-ReO_x/SiO₂ : A Combined Experimental and Theoretical Study

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Abstract

Recent advances in metabolic engineering have allowed to produce a wide range of platform molecules with variable numbers of carbon atoms, directly from the fermentation of biomass-derived aqueous sugars. Catalytic conversion of fermentation-derived 2-pyrone molecules has received considerable attention for the production of value-added chemicals [1]. In the present study hydrodeoxygenation of 2-pyrone molecule to jet fuel range n-alkane was carried out in the presence of silica-supported Ir-ReO_x catalysts in a single step without losing any carbon atom. The Re/Ir molar ratio of 0.5 exhibited maximum conversion (~99%) and selectivity (~83%) after 14 hours at 200 °C and 7 MPa H₂ pressure. Further, the catalyst was found stable even after four consecutive cycles with only 15 % loss in n-alkane selectivity. Selective synthesis of n-alkanes from 2-pyrones requires deep insights into the preference for the cleavage of C–O bonds for which density functional theory simulations were used to investigate hydrodeoxygenation of 2-pyrone on Ir–ReO_x, where ReO_x was dispersed on Ir. The Ir–ReO_x interface had a kinetic relevance in the ring-opening and deoxygenation steps whereas hydrogenation was derived by Ir. The comprehensive highlights reported here would guide the rational design of catalysts for the hydrodeoxygenation of cyclic esters.

Keywords: Biomass, 2-pyrone, bifunctional catalyst, density functional theory

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Degradation of E-Wastes using Carbohydrates in Water

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Abstract

E-waste represents the fastest-growing category of global solid waste with an increment rate of 30% per annum.¹ This complex waste consists of three main components; plastic, metals (precious and regular) and glass. E-waste would be used as a source of precious metals since mining of the same is anticipated to face significant challenges in meeting future demand.²

Sustainable recycling of the precious metals and the plastics from e-wastes using eco-friendly processes is challenging. In order to address this issue, carbohydrates are used to extract metals from the e-wastes; mainly using their extreme complexing ability with most of the metal ions. Simultaneously, trobichemical fragmentation of the plastic components of the e-wastes are carried out. The extent of the dissolution of the metals and other components are controlled upon changing the experimental condition. For example, the extraction of Cu, Zn, and Pb ions are most effective (in the supernatant) when D-glucose and urea are used. For Sn, the highest concentration is achieved when PCBs (an e-waste fragment) are treated with D-fructose in the presence of ammonium carbonate [(NH₄)₂CO₃]. Few more exciting results will be demonstrated during the presentation.

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Photosensitizer Loaded Lignin Nanoparticles for Treatment of Fungal Infection

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Abstract

Photodynamic therapy (PDT) has emerged as a promising clinical approach for treating Candida-induced infections. Compared to traditional antifungal treatments, PDT offers several advantages, including high effectiveness against pathogens, shorter treatment durations, precise targeting, increased specificity, and minimal toxicity to healthy cells. Previous research has shown that photosensitizers (PSs) loaded onto appropriate nanocarriers can enhance therapeutic effects. Metalloporphyrins, in particular, are important in PDT due to their capacity to produce reactive oxygen species (ROS) upon light activation. However, these macrocycles face challenges such as hydrophobicity, which can lead to aggregation and reduced biological effectiveness. In this study, a series of metalloporphyrins were designed and synthesized as phototherapeutic nanoagents. Theoretical calculations using Time-Dependent Density Functional Theory (TD-DFT) confirmed strong photosensitizing properties in these compounds. The metalloporphyrins were then incorporated into lignin to create nanophotocomposites, which provided hydrophilic and stable formulations. These nanophotocomposites exhibited significant singlet oxygen generation when exposed to green light, and they also demonstrated pH-responsive drug release. Upon green light irradiation, the nanophotocomposites showed a five-fold increase in PDT efficacy against *Candida albicans*. These newly developed phototherapeutic nanoagents show potential for treating oral and skin candidiasis.

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Ultra-Low Loaded Platinum Bonded Hexagonal Boron Nitride as Stable Electrocatalyst for Hydrogen Generation

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Abstract

Investigating catalyst loading's impact on intrinsic activity reveals a remarkable 5-fold increase in turnover frequency (TOF) when reducing Pt loading from 10^5 to 13 ngcm^{-2} , despite sluggish hydrogen evolution reaction (HER) in linear sweep voltammograms (LSVs) at lower loading.¹ Additionally, using a carbon matrix as a substrate introduces the drawback of carbon corrosion.² This study capitalizes on ultra-thin hexagonal boron nitride (hBN) layers' chemical stability in harsh electrolytes, leveraging nitrogen sites to stabilize platinum (Pt).³ The resulting HER catalyst, with low Pt loading (5 wt% or < 1 atomic%), demonstrates high intrinsic activity through Pt-N bonds with a non-zero Pt oxidation state. The Pt-N bonds are further confirmed through the X-Ray Absorption Studies(XAS) studies. Electronic modifications in shear-exfoliated hBN sheets are achieved via Au nanoparticle-based surface decoration (hBN_Au). Combining Au-decorated hBN with Pt forms the hBN_Au_Pt catalyst, which exhibits a significantly higher TOF for HER (~15 @ 50 mV overpotential) compared to the benchmarked Pt/C HER catalyst. Remarkably, the hBN_Au_Pt catalyst displays outstanding electrochemical and thermal stability, surviving an accelerated durability test of 10000 cycles (Overpotential enhancement of 7 mV @ 10 mAcm^{-2} current) and temperature annealing at 100°C . Density functional theory-based calculations align with experimental findings, affirming the vast potential of this novel catalyst system. This advancement effectively addresses concerns related to carbon corrosion and Pt leaching, marking a significant stride in electrochemical technology.

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Harnessing Localized Surface Plasmon Resonance in Ni₃N Nanosheets for Solar-Driven CO₂ Reduction

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Abstract

Surface plasmons have increasingly found applications within catalysis due to their charge carriers and enhanced product selectivity.¹ While the concept of plasmons has been long recognized, it has been predominantly limited to cost-intensive and less accessible metals such as Au, Ag, Cu, and Al. Building upon our ongoing research in catalysis, as documented in prior studies²⁻⁶, this investigation introduces hydroxy-terminated nickel nitride (Ni₃N) nanosheets as a promising alternative to the aforementioned metals for CO₂ hydrogenation. Remarkably, the Ni₃N nanosheets display a remarkable CO production rate (610 mmol g⁻¹ h⁻¹) and 99% selectivity toward CO under flow conditions utilizing visible light. Notably, when examining the photocatalytic reaction rates of excited plasmonic Ni₃N nanosheets, a super-linear power law (n) dependence on light intensity (I) is observed, with n = 6.3. This value significantly surpasses that of conventional plasmonic metal nanoparticles. Furthermore, the photocatalytic quantum efficiencies of Ni₃N nanosheets exhibit an augmentation with escalating light intensity and reaction temperature. The introduction of an electron acceptor, which serves as an alternative hot electron harvester, leads to a reduction in the rate of CO production, corroborating the involvement of a hot-electron mediated mechanism. Importantly, the thermal stability behavior of Ni₃N nanosheets provides critical insights into the non-thermal effects. Ni₃N nanosheets (which were thermally stable only up to 325 °C) showed stable catalytic activity for a long time (25 h), indicating that surface temperature must be below 325 °C during the plasmonic catalysis. Below this temperature, it showed poor catalytic activity in the dark. Additionally, in-situ DRIFTS studies shed light on the mechanism of CO₂ hydrogenation, revealing a direct dissociation pathway. In light of these findings, the exceptional catalytic performance exhibited by Ni₃N nanosheets underscores the potential of utilizing metal nitrides instead of traditional metal nanoparticles in the next generation of plasmonic photocatalysts.

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A Synergistic Approach for the Co-Production Of Hydrogen and Nanocarbon from Plastic Waste via Thermo-Catalytic Route

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Abstract

Thermo-chemical transformation of carbonaceous waste, such as plastics, emerges as a promising technology and a viable avenue to extract resources in contrast to conventional waste management methods like incineration and landfilling. Thermo-catalytic conversion of plastic waste to hydrogen is an innovative approach for addressing growing concerns of plastic pollution and the need for sustainable energy sources. Transition metals such as Ni and Fe over different supports such as Al_2O_3 , HZSM-5 can be used to convert plastic waste to hydrogen and nanocarbons. The hydrogen concentration in the Fe catalyst was slightly higher than that of nickel. In the case of nickel catalyst, more amounts of higher hydrocarbons and methane left the system unreacted due to the encapsulation of metallic Ni by carbon deposits and fast deactivation of the metallic, active phase associated with sintering. Raman spectra served to characterize the deposited carbon product. I_D/I_G ratio in case of Ni catalyst was higher with a value of 1.37 which confirms higher degree of graphitization while I_D/I_G ratio for Fe catalyst was 1.24. I_G/I_G ratio is higher in case of Fe catalyst than Ni which favours higher purity of deposited carbon. Carbon deposition was further evident from FESEM and HRTEM, which was indicated by the presence of filamentous carbons with a dense covering seen on the nickel catalyst surface, with most of the deposition being crooked or entangled.

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Banana Fibre Packaging Films as an Alternative Approach to Plastic: A Sustainable Approach

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Abstract

Banana fibre, generated as a waste material from the pseudo-stem of banana plant natural is a biodegradable material which has gained attention in recent times as a potential reinforcement in waste plastic recycling. Using banana fibre by blending it with different bio polymers can reduce the environmental impact by promoting the use of biodegradable components as a packaging material. Banana fibres were extracted from Musa Balbisiana species of banana through a fibre extractor machine. These fibres were degummed and then blended with chitosan, a bio-polymer and a packaging material was fabricated using solvent casting method. The films were characterized using several characterization techniques such as FT-IR, XRD, SEM, TGA and DSC. Mechanical property of the films were also calculated. Several functional tests such as swelling and degradation were carried out for extensive study of the packaging films. Our study shows that banana fibre-reinforced packaging films exhibit improved durability, thermal stability, and sustainability, making it a promising solution for reducing plastic waste while promoting circular economy practices.

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Enhancing Catalytic Efficiency: Co-Promoted Alumina-Supported Ni-Based Catalysts for NH₃ Decomposition

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Abstract

Hydrogen is key to global decarbonization, but storage and transportation are major challenges. On-site hydrogen production via NH₃ catalytic decomposition offers a promising solution ^{1,2}.



Though many studies emphasize the superior catalytic performance of Ru-based catalysts supported on different metal oxides, Ni based catalysts are viewed as the most cost-effective, option for the large scale. The objective of this study is to see the effect of Co as a promoter by tuning the Ni/Co ratio. We synthesize an alumina-supported monometallic (Ni/Al) and two bimetallic (NiCo/Al and Ni₃Co/Al) catalysts with a total metal loading of 12%, which are then characterized and tested for NH₃ decomposition. In the bimetallic catalysts, the Ni/Co ratios are 1 and 3 for NiCo/Al and Ni₃Co/Al, respectively. The oxidized and reduced catalysts are characterized using several techniques.

We achieve a significant improvement in catalytic performance when compared to the monometallic by tuning the Ni/Co ratio in the bimetallic catalyst. Notably, the catalyst with a Ni/Co ratio of 3 (Ni₃Co/Al) exhibits superior activity and stability. Characterization of the reduced catalysts confirms the presence of metallic Ni and Ni-Co alloys in monometallic and bimetallic catalysts.

The superior performance of the Ni₃Co/Al catalyst is due to its higher effective dispersion, formation of Ni-Co alloys, smaller particle size, and a larger effective surface area. **Tuning the Ni/Co ratio emerges as a key factor in driving this improvement in catalytic activity and stability.** These findings highlight the importance of alloy formation and dispersion control in optimizing catalyst performance for NH₃ decomposition.

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Enhancing Nucleation Understanding: Machine Learning Approach for Gas Hydrate Polymorph Classification

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Abstract

Understanding the kinetics and mechanisms of nucleation during crystallization is crucial for technological advancement. Molecular simulations play an important and complementary role to experiments by providing detailed molecular insights into nucleation processes. To analyze nucleation trajectories, crystalline order parameters are used to classify molecules into different phases, but designing these parameters is often complex and time-consuming. In this work, we focus on designing order parameters capable of identifying and classifying natural gas hydrates into different polymorphs. Starting from a set of generic order parameters¹, we systematically determine a minimal subset that can differentiate between water molecules in various polymorphs of gas hydrates, using machine learning principles. Specifically, we train the XGBoost² machine learning model to classify water molecules as belonging to liquid, ice-1h, ice-1c, sI, sII, or sH hydrates. This model is then applied to analyze methane hydrate nucleation near a planar gas-liquid water interface, with the nucleation rate calculated via the mean first passage time (MFPT) formalism³. Our model's performance is compared to previously developed order parameters from the literature⁴, showing that a minimal set of generic order parameters can accurately classify different crystal polymorphs, eliminating the need for developing specialized order parameters for each material under investigation.

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Data-Driven Design of Superior Electrocatalysts for the CO₂ Reduction Reaction Over Cu-based Alloys

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Abstract

The electrochemical reduction of CO₂ (eCO₂RR) offers a promising pathway for sustainable carbon capture and utilization by converting CO₂ into valuable chemicals and fuels.^{1,2} However, achieving efficient CO₂ conversion requires high-performance electrocatalysts capable of transforming the stable CO₂ molecule into useful products. While various electrocatalysts have shown selectivity for different chemicals, only copper-based electrocatalysts have demonstrated significant levels of C₂⁺ products. Other metals struggle with the crucial C-C coupling step necessary for forming C₂ products, and single-metal catalysts often fall short in achieving high selectivity for specific chemicals. Given the vast material space to explore experimentally, machine learning provides a faster and more cost-effective alternative for screening and optimizing catalysts.^{3,4} In this work, we introduce a comprehensive multi-scale approach using machine learning models to enhance and optimize the eCO₂RR process. Initially, we analyse experimental data to understand the effects of various components on a macro-scale process. Building upon these insights, we develop a molecular-scale model using density functional theory (DFT) data to explore the reaction mechanisms at the atomic level. This model helps identify suitable electrocatalysts by predicting reaction pathways and adsorption energies tailored for specific product selectivity. By integrating insights from both large-scale experimental data and theoretical analysis, our approach bridges the gap between empirical observations and theoretical predictions and further helps in the rational design of electrocatalysts.

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Removal of Sulfur Compounds from Fuels via Ternary Deep Eutectic Solvents

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Abstract

Transportation fuels like diesel consist of refractory organic sulfur compounds, the major contributors to environmental pollution, contributing to global warming. According to environmental legislation, a very low level of sulfur compounds is allowed in transportation fuels. Conventionally, refineries use a hydrodesulfurization (HDS) process, which requires high hydrogen pressure and high temperature, thereby increasing the cost of the process. Thus, there is a need for an alternative, cost-effective desulfurization process, which is the solvent extraction method, which requires ambient temperature and pressure along with a suitable solvent. Currently, researchers are paying attention to deep eutectic solvents (DESs) due to their versatile and tuneable properties in the desulfurization process. In this regard, a ternary DES was synthesized using metal halide, phenylacetic acid (PAA), and triethylene glycol (TEG) in the different mole ratios. The effect of DES was studied in the desulfurization of model fuels to optimize the mole ratios of DES. It was observed that the DES had found a sulfur removal efficiency of 50%. It can further be enhanced up to 97% via carrying multiple extractions (i.e., up to the fifth stage). Thus, the DES containing metal halides/ PAA/TEG can reduce the sulfur compounds from model fuel.

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High Rate Capability Dendrite Free Li -Ion Batteries using Fluorinated Carbon Thin Layers Modified Separators

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Abstract

Lithium metal batteries (LMBs) offer a great potential as an electrochemical energy storage solution for the future energy crisis due to their high theoretical capacity (3680 mAhg^{-1}) and low working potential of lithium anode (-3.04 V).^[1] However, major safety concerns arise from the uncontrolled lithium ion transport giving rise to dendritic growth and parasitic reactions such as continuous electrolyte degradation in the absence of a stable solid electrolyte interface (SEI) formation.^[2] To address these drawbacks, a facile and cost-effective approach for introducing a LiF/C-based artificial SEI using a novel fluorinated carbon thin layers modified separator membrane is proposed. The as-proposed SEI is formed during the cycling and improves the cell lifetime (lithium electroplating and stripping) by suppressing dendrite growth and inhibiting the electrolyte decomposition confirmed via post-cycling analyses such as scanning electron microscopy (SEM) and X-ray photoelectron spectroscopy (XPS). The galvanostatic cycling of Li/Li symmetric cell demonstrates an enhanced cycle life of >1500 cycles at a current density of 3 mAcm^{-2} over the unmodified cells (50 cycles) with a similar range of over potential ($\sim 0.25 \text{ V}$). Similar trend is observed at a very high current density of 10 mA cm^{-2} that makes the fluoro carbon modified separator highly compatible to be used for high power-density applications. The commercial applicability of the modification is further supported by the LiFePO_4 based full cell studies. The studies further opens up the possibilities of the extension of such LiF/C rich SEI for the solid state electrolytes as well.

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Design of Scale up Process for Batch Synthesis of Polyether Sulfone (PES)

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Abstract

Epoxy composites find application in defense and space applications. Brittle nature of these composites limits their application. To overcome this and to extend its applicability to defense and space, thermoplastic tougheners are added to the epoxy. Polyether sulfone (PES) has been more commonly used as a toughener for epoxy due to its modulus, toughness, high glass transition temperature (T_g), chemical resistance and high thermal stability. The commercial availability of this in India is limited. Indigenous technology for the manufacture of PES has not been developed. To develop the technology for lab scale synthesis of PES, a nucleophilic aromatic substitution reaction was implemented to produce 1 g of this material. The structural characteristics of the material was confirmed by ¹H-NMR and FTIR. Thermal analysis was done to confirm its thermal stability by TGA and DSC. Other characterizations like XPS, XRD, CHNS analysis were performed to confirm the elements present in the material. The morphological studies were obtained using FE-SEM. The process was then scaled up to produce 100 g of the material and thereby to two kg of the material using a 20 L capacity reactor assembly with condenser and other accessories was designed. The product synthesized by using 2 kg bulk reactor assembly was characterized and was found to have similar characteristics as the one gram and 100 g batch.

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Degradation and Conversion of Plastic Waste into Secondary Resource Materials

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Abstract

The effective management of plastic waste (PW) is crucial for achieving environmental sustainability. Plastic waste, a significant component of municipal solid waste (MSW), poses severe ecological threats if not properly segregated and disposed of. It takes more than 200–500 years for plastic to degrade, and a large portion ends up in landfills and marine environments. These polymers eventually break down into secondary pollutants like microplastics (<5mm) and nano plastics (<0.1 μm), which can disrupt the food chain by absorbing harmful contaminants. This study explores the in-situ photochemical degradation of plastic wastes, specifically low-density polyethylene (LDPE) and high-density polyethylene (HDPE), into resourceful materials. A photochemical reactor is employed for degradation using UV-A light, with parameters such as pH, catalysts, light intensity, time, and temperature optimized for maximum efficiency. After degradation, the material undergoes chemical treatment through an oxidation process to obtain secondary raw materials for sustainable applications, which holds significant applications in the production of nylon, resins, plasticizers, and polyurethane foam, further enhancing the value of the degraded plastic. This approach provides a viable pathway for transforming plastic waste into resourceful industrial materials.

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Covalent Organic Framework Impregnated with Silver and Copper Nanoparticles: An Advanced Approach for Catalytic Degradation of Organic Pollutants in Wastewater

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Abstract

In this study, we present an economically viable and scalable method for synthesizing a novel covalent organic framework (COF), TzTFB-COF, a nitrogen-rich cross-linked polymer. TzTFB-COF is synthesized using s-tetrazine diamine (Tz) and 1,3,5-triformylbenzene (TFB) as building blocks, yielding a material with high chemical and thermal stability ($>300\text{ }^{\circ}\text{C}$). Functionalization with silver and copper nanoparticles via solution infiltration results in Ag@TzTFB-COF and Cu@TzTFB-COF composites, characterized by high thermal stability up to $350\text{ }^{\circ}\text{C}$, and metal contents of 9.6 wt% and 12.4 wt%, respectively, as determined by ICP-OES. These composites exhibit excellent catalytic activity, selectivity, and reusability in the hydrogenation of nitroaromatic compounds (NACs) in aqueous media. Catalytic performance is highlighted by rate constants of 0.0185 s^{-1} and 0.0219 s^{-1} and Gibbs free energies of 9.878 kJ/mol and 9.615 kJ/mol for Ag@TzTFB-COF and Cu@TzTFB-COF, respectively, indicating endothermic, endergonic, and nonspontaneous reaction characteristics. The promising results underscore the potential of these metal-functionalized COFs as efficient, stable, and reusable catalysts for environmental applications involving the degradation of hazardous NACs.

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A Combined Experimental and Theoretical Approach to Investigate the Role of Molybdenum Oxide (Molybdena) as a Promoter for Propane Dehydrogenation Reaction over ZrO₂ Supported Vanadia Catalyst

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Abstract

Supported vanadia oxides (vanadia) serve as one of the potential catalysts for direct dehydrogenation (DH) of propane because of their high reactivity [1,2]. However, investigations probing the role of a secondary inactive metal oxide as a promoter for propane DH are limited [3]. Here, we investigate the promotional behaviour shown by molybdenum oxide (molybdena) as a secondary metal oxide that is relatively inactive for the propane DH reaction using both theory and experiments. Raman spectroscopy, H₂-TPR and XPS results reveal that both molybdena and vanadia are present as molecularly dispersed moieties, VO_y and MoO_x, and when they are simultaneously present, they do not exhibit any interactive behaviour, which is confirmed by density functional theory (DFT) calculations. However, reactivity studies reveal that the propane conversion and propene yield are enhanced when VO_y and MoO_x are simultaneously present. Several parameters, such as: (a) oxygen vacancy formation energy, (b) propane adsorption and dissociation energies on VO_y and MoO_x, (c) one hydrogen adsorption energies, and (d) two hydrogen (2H) adsorption energies are studied in depth by DFT to understand the promotional effect shown by MoO_x. Our findings suggest that the VO_y and MoO_x moieties behave independently except for the last parameter. In the case of 2H adsorption the presence of MoO_x alongside VO_y makes the adsorption process thermodynamically favourable. As propylene is obtained by abstracting two hydrogen atoms, applying the BEP relation we can infer that MoO_x moiety lowers the barrier required for removing the second hydrogen thereby explaining its promotional behaviour.

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Tailoring Catalyst for Selective Guar Gum Conversion: Unveiling the Interplay between Structure and Surface Functionalities in Galactose and Mannose Production

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Abstract

In this work, we present an efficient catalytic approach for the hydrolysis of galactomannan bonds in guar gum to produce galactose and mannose. The functional carbon catalyst, designed with surface functionalities and structural features through post-treatment, demonstrated enhanced glycosidic bond hydrolysis. Advanced characterization techniques, including X-ray photoelectron and Raman spectroscopy, confirmed the modified catalyst's active binding sites and its interaction with guar gum through its amorphous nature. Under optimized conditions, a high selectivity of 90% mannose and galactose was achieved on total conversion. The catalyst exhibited robust performance, maintaining activity and stability across four cycles, making it a promising candidate for industrial applications.

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Chemically-Functionalized MoS₂/WS₂ Heterostructure: A Novel Lubricious Material to Decrease Energy Consumption by Minimizing the Frictional Losses for Engineering Surfaces

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Abstract

Rising concerns about energy conservation and environmental sustainability have recently intensified global efforts, particularly the design of novel nanostructured materials, to develop energy-efficient and environmentally benign lubricants for transportation and industrial processes.^{1,2} The 2D heterostructure with dissimilar lattice constants can significantly influence interfacial interactions, leading to a remarkably low coefficient of friction for enhanced lubrication performance.³ The current study explores the synthesis and lubrication aspects of chemically functionalized dichalcogenides (cf-MoS₂/WS₂) heterostructure, which not only furnished the unique properties of MoS₂ and WS₂ but also addressed the synergistically low coefficient of friction to minimize the energy losses. The cf-MoS₂/WS₂ heterostructure was synthesized by hydrothermal growth of MoS₂ on the exfoliated ultrathin sheets of WS₂ in the presence of cationic surfactant. The cf-MoS₂/WS₂ heterostructure demonstrated stable dispersion in SN 500 base oil. The comprehensive analyses, including FTIR, Raman, XRD, TGA, XPS, and HRTEM measurements, revealed the chemical, structural, crystalline, and morphological features of cf-MoS₂/WS₂. An optimized dose of cf-MoS₂/WS₂ heterostructures in SN 500 base oil (0.2 mg/mL) led to a 51% and 69% reduction in friction and wear for steel tribo-pair. Moreover, cf-MoS₂/WS₂ heterostructures showed significantly better tribo-performance compared to the MoS₂ and WS₂ under identical conditions, attributing to the interfacial lattice mismatch derived from the difference in the lattice constants of MoS₂ and WS₂ in cf-MoS₂/WS₂ heterostructures. The Raman spectroscopy and EDS analyses of the worn scars further confirmed the deposition of cf-MoS₂/WS₂-based thin film on the tribological interfaces, validating the enhanced performance of SN 500 oil. Moreover, post tribo tests, the Raman and XRD analyses of residual heterostructure confirmed the exceptional stability of cf-MoS₂/WS₂ throughout the test.

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Nano-Scale Wonders: Amine Carbon Quantum Dots as Next-Gen Catalysts

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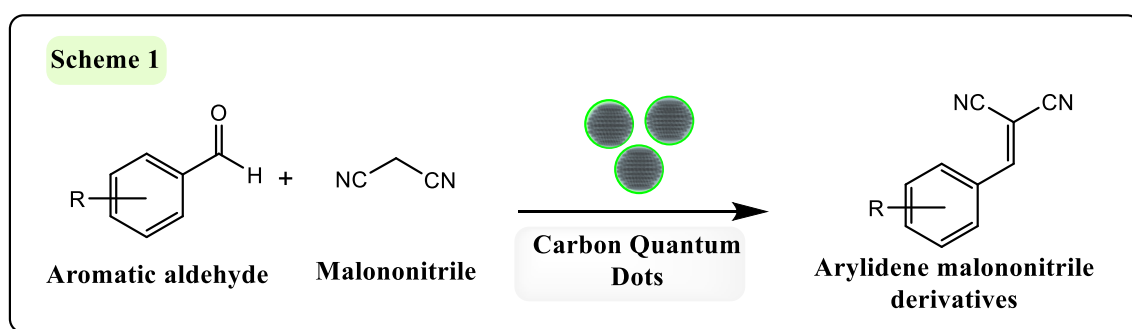
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Abstract

Carbon Quantum Dots (CQDs) have been extensively studied in recent years.¹ The gaining interest is due to the unique properties such as bright fluorescence², excellent photostability³, tuneable fluorescence emission⁴, biocompatibility, low toxicity, and good water dispersibility. Carbon dots with a well-tuned surface can be used for applications such as catalysis¹, bioimaging, biosensing, etc.

This work prepared and purified CQDs from diethylenetriamine (DETA-CQD). The amine-functionalized DETA-CQD was applied as a catalyst for the Knoevenagel condensation reaction (Scheme 1). The synthesized CQDs exhibited excellent catalytic activity for the model Knoevenagel reaction between benzaldehyde and malononitrile, compared to inorganic bases and amine catalysts. The CQDs exhibited high conversion rates, excellent selectivity, and recyclability due to their high surface area, and the presence of abundant surface functional groups. The CQDs demonstrated excellent compatibility with various functional groups and substrates, making them versatile catalysts for a wide range of organic transformations. The nature of the nanomaterial facilitated easy separation and recovery, contributing to the sustainability and cost-effectiveness of the catalytic process.⁵



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Construction of LDH-derived Bimetallic Metal-Organic Framework (BMOF) with Defect Engineering for High-performance Supercapattery Application

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Abstract

Developing a bimetallic metal-organic framework is crucial for advancing energy conversion and storage technology. However, the tendency of the bimetallic-MOF materials to agglomerate easily during synthesis generally impedes their direct application as electrode materials. Herein, our study has introduced a method for synthesizing bimetallic NiMn-MOF through an in-situ transformation from NiMn-layered double hydroxide (LDH) array. This approach has demonstrated significant adaptability with the development of defect-engineered MOFs, which can efficiently adjust the electronic structure of the metal center, resulting in improved electrochemical performance as an energy-storage material (supercapattery) with a storage capacity of 532 C/g and was able to outperform the energy storage capacity of scaffold NiMn-LDH (423 C/g) and Direct NiMn MOF (258 C/g) synthesis routes. In addition, an aqueous asymmetric supercapattery device was assembled using LDH-D NiMn-MOF as the positive electrode and Fe₂O₃/Fe₃O₄/CNF as the negative electrode (previously synthesized in our laboratory), resulting in a maximum energy density of 55.99 Wh kg⁻¹ and power density of 6.83 KW kg⁻¹ and maintained 94.4% of its original capacitance after 6000 continuous cycles at a current density of 10 mA cm⁻². Therefore, the development of the LDH-derived bimetallic metal-organic framework underscores its potential for sustainable energy storage applications in the future.

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Iron Single-Atom Catalysis: A Sustainable Route to DFF from HMF on Nitrogen-Doped Graphene Acid

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Abstract

Transforming 5-hydroxymethylfurfural (HMF) into the valuable biobased product, 2,5-diformylfuran (DFF), using non-noble metal catalysts has been a persistent challenge. To address this, we developed a single-atom iron catalyst supported on nitrogen-doped acidic graphene (Fe₁-NGA), which showed outstanding efficiency in the oxidation of HMF. The interaction between iron atoms and the graphene surface led to a partial reduction of Fe³⁺ to Fe²⁺ due to charge transfer with the graphene's acidic functional groups. This unique combination of Fe³⁺ and Fe²⁺ was key in driving the catalytic process, enabling both high HMF conversion and selective DFF formation. Under carefully optimized alkaline conditions, the Fe₁-NGA catalyst achieved nearly complete conversion of HMF with a DFF selectivity of 92%, maintaining stable performance with minimal loss over time. Furthermore, the catalyst proved highly durable, showing no significant aggregation or deactivation after three consecutive cycles. This work highlights the potential of single-atom catalysts on functionalized graphene as a promising route for efficient and sustainable biomass conversions, offering a viable alternative to conventional noble-metal-based systems.

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Ossified Zinc Alendronate Catalyst for Glycerol Valorization Using Urea as CO₂-Surrogate

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Abstract

The production of a variety of functional moieties of industrial importance from CO₂, a molecule with relatively low reactivity, is a challenging subject. According to the Global Opportunity Analysis and Industry Forecast, 2022-2031, the biodiesel market accounted for 2,781.0 million in 2021 and is anticipated to reach 3,579.1 million in 2031, with a CAGR of 2.6%[1]. The refined glycerol segment held the largest market share with 77.1%[2]. This presents a substantial opportunity for the use of glycerol as an alternative and sustainable feedstock for many chemical intermediates. Organic carbonates such as glycerol carbonates are essential commodity chemicals due to their extensive application and growing demands as chemical intermediates, especially as polymer building blocks[3]. Using urea as a CO₂-surrogate, glycerol carbonate can be synthesized from glycerol, obtained as a by-product or waste from the oleochemicals industry, thereby promoting the integrated bio-refinery cause. Ossified zinc alendronate catalyst materials have demonstrated high activity in the reaction of glycerol to glycerol carbonate using urea. Detailed investigations of the catalyst materials suggest that both basic and acidic sites within the catalyst system contribute to the outstanding activity. The glycerol and urea molecules are activated by basic and acidic sites on the same catalyst, respectively.

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Catalytic Asymmetric Fragmentation of Cyclopropane

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Abstract

The activation of alkanes in a stereoselective manner has long posed a significant challenge in chemistry. Although metal-containing enzymes can oxidize alkanes with impressive ease and selectivity, chemical methods have traditionally been restricted to transition metal-based catalytic C–H functionalizations. A known method for alkane cracking involves the protonation of alkanes to generate pentacoordinated carbonium ions, which can then be fragmented into smaller hydrocarbons in the presence of strong Brønsted acids. Despite this, achieving catalytic stereocontrol in such reactions has been elusive. In this study, we demonstrate that using strong and confined acids can catalyze highly enantioselective fragmentations of various cyclopropanes, leading to the formation of the corresponding alkenes. This approach represents a significant advancement in the field of catalytic selective alkane activation.

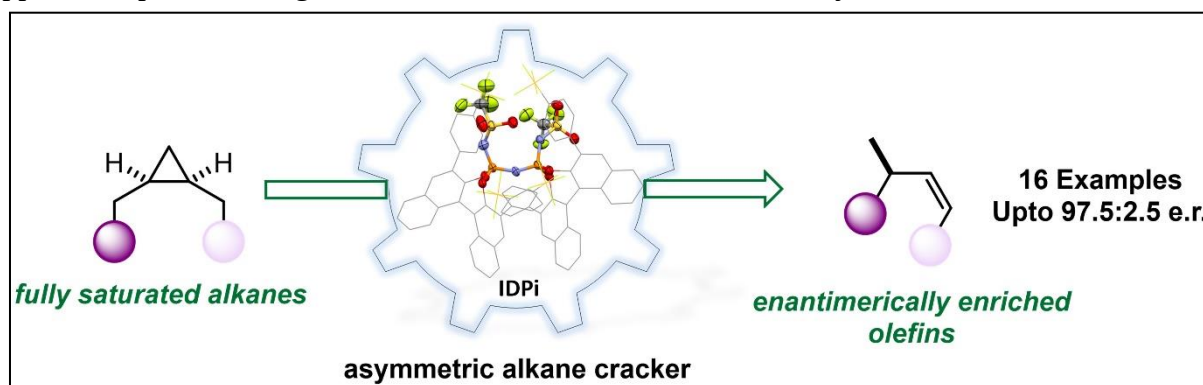


Fig. 1. enantioselective fragmentation of cyclopropane by IDPi catalyst.

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Enhancing Iodine Capture with Electrospun Nanofiber-Supported Covalent Organic Frameworks

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Abstract

Covalent organic frameworks (COFs) have emerged as state-of-the-art sorbents for iodine capture, demonstrating exceptional sorption capacities exceeding 10 g/g with rapid kinetics and excellent recyclability.[1] This intriguing behaviour often stems from their high surface areas, controllable pore-interface and structural tunability.[2] Despite advancements, the influence of particle size and morphology control in COFs has been overlooked in the literature. Recognising the research gap, we developed a series of imine-linked isostructural COFs with distinct particle sizes and morphologies to enhance their iodine sorption behaviour. Our study demonstrates that solid-state aggregation in powdered form limits the sorption efficacy of nano/mesoCOFs while passivating their external surfaces. To overcome this challenge, we supported these COFs on electrospun nanofibrous membranes with an in-situ growth strategy. This strategy, coupled with rapid mass transfer, faster sorption kinetics, accessible binding sites, improved processability, and enhanced chemisorption, guiding the development of next-generation iodine sorbents.

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Solar Light Driven Acetylene Semi Hydrogenation using Plasmonic Black Gold

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Abstract

In general, catalysts for reduction are unstable in the presence of air. A plasmonic reduction catalyst that is stable only in air has been described in this work. A highly active, selective and particularly air-stable plasmonic reduction catalyst for acetylene semi-hydrogenation was developed by loading Pt-doped Ru nanoparticles¹ on 'dendritic plasmonic colloidosomes (DPC)', also known as black gold². With over 90% selectivity and ethene productivity of 320 mmol g⁻¹ h⁻¹ of ethene, the DPC/RuPt catalyst outperformed nearly all previously reported catalysts. The critical role of co-existing metal oxide and metal phase was evidenced by high catalytic activity and long-term stability for at least 100 h, which could only be achieved by providing continuous airflow along with the reactant feed.³ Plasmon-mediated simultaneous reduction and oxidation of the active site during the reaction were responsible for the unprecedented stability of the catalyst which was demonstrated by various spectroscopic analyses (XPS, EXAFS, and XANES). FDTD simulations showed a five-fold enhancement in the electric field as compared to pristine DPC due to the near-field coupling between the RuPt nanoparticles and DPC. The KIE measured in light was larger than in the dark at all temperatures, implying the contribution from the non-thermal effects along with the photothermal activation of the reactants as a result of plasmonic activation.^{4,5} In-situ FTIR studies provided insight into the molecular reaction mechanism over the oxide surface and highlighted the role of the intermediates in determining selectivity. The integration of advanced spectroscopic techniques and simulations provided deep insights into the catalyst's behavior and mechanism, showcasing its potential for practical applications in sustainable catalysis.

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Quest for Desolvated Structure Unveils Breathing Phenomena in a MOF: Greener Complete Organic Transformations

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Abstract

Robust metal-organic frameworks (MOFs) with open metal sites provide excellent platform for Lewis acid catalysis.[1] The crystal structure of MOF, $\{Mn_2(1,4-bdc)_2(DMF)_2\}_n$ is known for long time, however, its desolvated structure, $\{Mn_2(1,4-bdc)_2\}_n$ (Mn-BDCdesolv) is not yet known.[2] The first principles-based computational simulation was used to unveil the structure of Mn-BDCdesolv. We have used Mn-BDCdesolv in cyanosilylation reaction and recorded up to 99.9% conversions with 8 aldehydes.[3,4] These results inspired us to use Mn-BDCdesolv in cyanosilylation reactions in solvent-free conditions and our experiments show 99.9% conversions with 20 aldehydes.[5] The catalyst also provided 99.9% conversions in CO₂ cycloaddition reaction with various epoxides. Further, in Knoevenagel condensation, Mn-BDCdesolv provides 99.9% conversions of 16 aldehydes with TON up to 16650. We extended its application to C-N bond formation. Mn-BDCdesolv exhibited remarkable conversion up to 99.9% in benzimidazole synthesis and Strecker reaction with TON up to 8250, benzoxazole synthesis with TON up to 4409. Mn-BDCdesolv demonstrated excellent recyclability up to 24 and 30 cycles in Knoevenagel condensation and benzimidazole synthesis, respectively. Our investigations illustrate that Mn-BDCdesolv (i) is economical, efficient and robust catalyst that enables solvent-free greener set-up, satisfying some principles of green chemistry and therefore catalysis with Mn-BDCdesolv can be regarded as "green catalysis"

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Catalytic Methane Dissociation and its Non-Oxidative Coupling in Metal-Dispersed Molten Salt media: An Ab Initio Molecular Dynamics Investigation

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Abstract

Methane dehydrogenation in molten media is an emerging technology for producing CO₂-free hydrogen and solid carbon^{1,2}. Furthermore, the non-oxidative coupling of methane (NOCM) generates more valuable C₂ products, along with H₂. Molten salts, as a potential molten medium, exhibit weak catalytic activity for methane activation. The catalytic activity of molten salts and their selectivity for C-C coupling can be enhanced by dispersing active metals into the molten salt. Our research focuses on methane dehydrogenation and NOCM reactions using Car-Parrinello Molecular Dynamics simulations in various metal-dispersed (Ni, NiB, Cu, and CuB) molten salt (NaBr) systems. We found that at high temperatures, the agglomeration of Cu atoms enhances the activity of Cu catalysts for CH₄ activation, while boron doping in Ni and Cu catalysts improves their activity through surface reconstruction. Our simulations revealed that the CuB-NaBr system uniquely promotes non-oxidative C-C coupling reactions over the competing dehydrogenation of intermediates, whereas other metal-dispersed systems primarily favor complete CH₄ dehydrogenation. Carbon generated as a byproduct diffuses into Ni and Cu, leading to deactivation, but boron-doped systems prevent this diffusion, making them promising candidates for avoiding catalyst deactivation. These findings facilitate the development of stable, active molten mediums for producing C₂ products and H₂ from natural gas.

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Machine Learning Accelerated Density Functional Theory-Based Investigation of CO₂ Hydrogenation to Ethanol on Ni and Boron-Doped Ni Surfaces

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Abstract

Ethanol synthesis from CO₂ can mitigate global warming by converting a greenhouse gas into a valuable fuel. However, this requires an efficient catalyst. While Ni activates CO₂, it predominantly hydrogenates it into methane.[1] Studies have shown that boron doping in transition metals facilitates the C-C coupling.[2] The impact of boron doping in Ni on CO₂ hydrogenation to ethanol can be better understood by density functional theory (DFT) as it provides atomic-level insights that are not easily accessible through experimental approaches, helping to tune the catalyst performance. However, since DFT simulations are computationally expensive and there are 150 elementary reactions involved, making DFT alone impractical, we used a machine learning (ML) approach to expedite the process. Our ML model was trained using DFT data from literature and our simulations, correlating activation energy with descriptors like reaction energy, reaction characteristics (type, reactants, products), catalytic surface, and computational setup.[3] Among the regressor models employed - random forest regressor (RFR), gradient boost regressor, and support vector regressor - RFR predicted the activation barrier most accurately, with a mean square error of 0.0741 eV. The DFT-ML results revealed that boron incorporation significantly reduced the C-C coupling barrier, suggesting that NiB could be a promising catalyst for ethanol synthesis.

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Computational Study of Electronic Structure of Magic-Sized CdSe Quantum Dots and Charge Transfer Dynamics in CdSe QD-Carbazole Systems

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Abstract

Photoluminescent semiconducting cadmium selenide (CdSe) quantum dots exhibit unique optical properties.[1] Their emission wavelength can be precisely tuned by varying their size, and utilizing them in essential applications. In recent years, magic-sized tetrahedral shaped CdSe quantum dots have been precisely synthesized, and their optical properties have been evaluated.[2] In this work, we computationally studied the electronic structures of tetrahedral-shaped CdSe QDs and examined the photoexcited charge transfer process in QD-molecule systems. All the simulations were performed with the DFTB+ package.[3] The electronic structure of these T1, T2 and T3 CdSe QDs was determined by using the self-consistent charge density functional tight-binding (SCC DFTB) method .[4] We modelled ultrasmall, atomically precise tetrahedral CdSe QDs i.e., Cd₃₅Se₂₀X₃₀L₃₀ (T1), Cd₅₆Se₃₅X₄₂L₄₂ (T2), and Cd₈₄Se₅₆X₅₆L₅₆ (T3) with different sizes (average edge length ranging from 1.65 nm to 2.49 nm) and uniform composition of ligands where X=CN, L=NH₃. Performing electron dynamical simulation, we computed the absorption spectra, revealing the lowest energy transitions at 3.85 eV for T1, 3.61 eV for T2, and 3.47 eV for T3. The overall absorption spectra are red-shifted with increasing the size of QDs from T1 to T3, exhibiting a quantum confinement effect. Our calculated spectra are qualitatively agreed with the experimentally measured values.[5] Furthermore, we investigated the charge transfer dynamics in CdSe QD-carbazole models. The amino group of carbazole attached to the apex position of tetrahedral QDs. Three models were constructed depending on the position of amino group attached to the carbazole i.e., T1-2A-Cz, T1-3A-Cz, and T1-4A-Cz. We investigated the charge transfer dynamics of these T1-Cz models by employing a time-dependent sinusoidal perturbation. Among these, T1-3A-Cz shows an ultrafast charge separation within the femtosecond timescale due to the effective hole delocalization between T1 QD and 3-amino carbazole. While other positions of carbazole did not show efficient charge separation. So, the T1-3A-Cz model acts as a perfect donor-acceptor QD-molecule nanocomposite that can harvest photon energy efficiently. In T2-carbazole systems, the photoinduced charge transfer is negligible because of weak electronic coupling, and it is not detected in T3-carbazole systems. [6]

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DFT-Guided Design of Catalysts for the Conversion of Biomass-Derived Furfural to Furfuryl Alcohol

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Abstract

The conversion of biomass into value-added chemicals is key area of focus in sustainable chemistry and engineering. Furfural (FCHO), obtained from biomass through the acid-catalysed dehydration of xylose (a major component of hemicellulose in lignocellulose), plays a key role in this process. About 65% of the global production of furfural is converted into furfuryl alcohol (FCH₂OH), which is widely used in resins, potential fuels etc. However, the incomplete understanding of the reaction mechanisms on various metal catalysts often leads to unwanted decarbonylation reactions, forming furan, which hinders efficient conversion.

To address this, we employed Density Functional Theory (DFT) calculations to investigate the reaction mechanisms of FCHO to FCH₂OH on four transition metal surfaces: Pd (111), Ni (111), Pt (111), and Cu (111). Our findings indicate that the preferred pathway to FCH₂OH involves the FCHOH intermediate on Pd (111), Ni (111), and Pt (111) surfaces, while on Cu (111), the pathway proceeds through the FCH₂O intermediate. The reaction barrier for this pathway on Cu (111) is 0.77 eV, lower than the barriers for FCHOH formation on Pd (111), Ni (111), and Pt (111). Additionally, the binding energy of FCH₂OH on Cu (111) is -1.17 eV, significantly lower than the ~-2 eV observed on the other three surfaces. Copper-based catalysts enhance FCH₂OH selectivity, minimizing undesirable decarbonylation products.

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Unravelling the Mechanochromic Luminescence and TADF Relationship in Metal-Free Organic Material

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Abstract

Metal-free organic emitters with thermally activated delayed fluorescence (TADF) properties are promising for organic light-emitting diodes (OLEDs).[1] The TADF process depends on efficient reverse intersystem crossing (RISC) to convert triplet into singlet states. Takeda and co-workers discovered that the U-shaped PTZ-DBPHZ-PTZ triad shows multicolour emissions with mechanochromic luminescence (MCL) and TADF properties, which can switch from a localized exciton (LE) state to a charge-transfer (CT) state, exhibiting substantial TADF character.[2] We computationally investigated the structure-property relationships of the D-A-D triad conformers (i.e., Axial-Axial (AA), Axial-Equatorial (AE), and Equatorial-Equatorial (EE) conformers) using time-dependent density functional theory (TDDFT) with range-separated hybrid functionals (CAMY-B3LYP) and TZP basis sets, considering scalar relativistic effects with the zero-order regular approximation (ZORA).[3-4] Our calculations revealed that the EE conformer shows TADF properties due to close spacing and effective crossing between 3LE1A, 3CT1, and 1CT1 states, enabling efficient harvesting of triplet CT to the S1 state ($3CT1 \rightarrow 1CT1$) with sufficient RISC ($\sim 10^7$ s⁻¹). Calculated fluorescence and intersystem crossing (ISC) rate constants indicate that prompt fluorescence is active for AA conformers but inactive for others.[5] Our study elucidates the tunable luminescence characteristics of the D-A-D triad, aiding the rational design of TADF materials.

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Photoexcited Electron Transfer in Zn Porphyrin–Nanographene Composites

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Abstract

Photoexcited charge transfer is crucial in solar cells and photocatalysis. [1][2] This work is about modelling donor-acceptor systems consisting of Zn-porphyrin (ZnP) and polyaromatic hydrocarbons PAH, which can be considered nanographenes (NG). Electron-rich macrocycles such as porphyrin are used in photoexcited electron transfer and are excellent photosensitizers.[3][4] End functionalization of the NG with diimide can result in exotic electronic and charge transfer properties. They can be used in optoelectronic devices.[5] We used density functional theory with the hybrid density functional ω B97X-D and 6-31+G (d, p) basis set. The excited state properties were performed with time-dependent DFT (TD-DFT). The fragment charge difference (FCD) method was used to calculate the electronic coupling between bright and charge transfer states. All these calculations were performed with the Q-Chem-5.4 package. The Marcus theory of electron transfer was used to calculate the charge separation rate in ZnP–NG systems. In the extension of the size of the nanographene, the ZnP-CO-NG1 and ZnP-CO-NG2 (where CO denotes the carbonyl linkage) donor-acceptor models displayed a high rate compared to ZnP-CO-NG3. Altering the linkers in ZnP-L-NG1, the system acetylene and benzene linkages showed a higher CT rate constant. In the case of ZnP-L-NG2, acetylene and benzene linkers did not improve the CT rate more than ZnP-CO-NG2. Again, in the case of ZnP-L-NG3, acetylene improved the CT rate more than ZnP-CO-NG3. This work demonstrated how the acceptors' size and different linkers affect the charge separation between ZnP and NG.

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Metal Borides Supported Graphitic Carbon Nitride as Non-Noble Catalytic Materials for Transfer Hydrogenation of Nitroarenes

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Abstract

The reduction of nitroarenes to their corresponding aromatic amines is one of the most frequently occurring reactions in chemical synthesis. However, traditionally molecular hydrogen (H_2) was used to hydrogenate organic compounds, but this method has some limitations, such as the highly flammable nature of H_2 , the need for high temperatures, and the handling of high-pressurized H_2 . The catalytic transfer hydrogenation (CTH) approach has captured the interest of researchers as an affordable and ecologically friendly alternative to traditional hydrogenation methods. In this work, metal borides are used as effective catalysts for hydrogenation reactions due to their ability to create active hydrogen species required for the desired reaction. This study investigates the hydrogenation potential of nickel boride (Ni_3B) for the transfer hydrogenation of aromatic nitro compounds with hydrazine hydrate as the hydrogen source. Graphitic carbon nitride (GCN) was used to support Ni_3B , allowing for more active reaction sites. The Ni_3B -GCN catalyst shown high catalytic potential for hydrogenating nitro compounds to amines, achieving 100% conversion efficiency and yields. By changing various reaction parameters, such as time, temperature, solvents, catalyst amount, and hydrogen sources, the reaction conditions were optimised. A comprehensive analysis of the as-synthesized catalysts has been conducted using various characterization techniques. The utilization of efficient Ni_3B -GCN catalysts for hydrogenation processes could open the way for sustainable and successful industrial organic catalysis.

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Mechanistic Study of Ethane Oxidative Dehydrogenation with CO₂ over Molybdenum Carbide Catalysts

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Abstract

CO₂-assisted Oxidative Dehydrogenation (CO₂-ODH) of ethane is a promising alternative to the existing methods for ethylene synthesis. We present DFT simulations based mechanistic details of ethane CO₂-ODH over β -Mo₂C catalyst. In the absence of oxidant CO₂, the C-H activation in ethane was highly unfavorable with extremely high barriers, indicating that the Mo-C site pairs on β -Mo₂C(101) surface are not the most active ODH sites. The comparatively low CO₂ dissociation barrier on β -Mo₂C(101) leads to surface oxidation during ethane ODH. Ab initio thermodynamics calculations suggested a fully oxygen covered β -Mo₂C(101) surface at typical ODH conditions. On this surface, C-H activation in ethane by adsorbed O has a lower activation barrier but results in the favorable formation of ethoxide and acetaldehyde intermediates, leading to low ethylene selectivity. Upon deeper surface oxidation and formation of surface MoO₂ layers, the formation of oxygenated derivatives was not observed, indicating improved ethylene selectivity. The C-H activation barrier in ethane over the Mo-O sites is comparatively lower and the CO₂ activation barrier became comparable to that of ethane activation, suggesting the approach to steady state. This MoO₂ oxide overlayer on Mo₂C is likely to be a selective catalyst for CO₂-ODH of ethane to give ethylene.

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Tuning Singlet-Triplet Energy Gap in Donor-Spacer-Acceptor based TADF Emitters - A DFT Study

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Abstract

The tuning of the singlet-triplet energy gap is an active area of research in the development of Thermally Activated Delayed Fluorescence Organic Light Emitting Diodes (TADF-OLEDs),¹ a promising technology increasingly used in commercial multi-colour display applications². The singlet-triplet energy gap is influenced by the exchange energy, which in turn depends on the choice of donor/acceptor pair, the type of linkage, as well as the distance and torsion angle between the donor (D) and acceptor (A).^{3,4,5} This study focuses on screening a D-spacer-A system with various spacers, through systematic structure-property relationship studies, to identify the one that yields the lowest singlet-triplet energy gap using DFT and TDDFT calculations. Various linkers with varying distances and torsion angles have been tested. Additionally, the impact of various electron-donating and withdrawing substituents on the spacer linked donor and acceptor moieties, was investigated in vacuum and solvents of varying polarities. The results were analysed to identify the best emitter having the lowest singlet-triplet energy gap. These findings will contribute to the efficient design of D-S-A molecules for future TADF-OLED applications.

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Elucidating the Role of Metal-Solvent Interface in the Hydrogenation of Maleic Acid to Succinic Acid: A DFT Study

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Abstract

Performing reactions at the metal/solvent interface are central to the process of biomass upgradation to value added fuels and chemicals. The type of solvent used significantly affects the kinetics and thermodynamics of the reaction, thereby altering the conversion and selectivity. Screening of desired solvent experimentally is accompanied by consumption of time and resources which can be cut down by using computational tools. Furthermore, experimental techniques cannot be employed easily to understand the metal/solvent interaction at the molecular level. Several studies have examined the impact of solvents on the hydrogenation of C=O bonds, but there are only a limited number of studies that focus specifically on the hydrogenation of C=C bonds. This study aims to investigate the fundamental understanding of solvent effect in C=C bond hydrogenation by considering hydrogenation of maleic acid to succinic acid on Pd (111) catalyst surface as a model reaction, using ab-initio Molecular Dynamics (AIMD) and Density Functional Theory (DFT) simulations.

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Computational Insights into the Adsorption Behavior of H₂ And CO₂ on Cu And ZnO Surfaces for Methanol Synthesis

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Abstract

Cu-based catalysts are widely studied for CO₂ hydrogenation to methanol, providing a dual benefit of reducing CO₂ emissions and producing valuable methanol^[1]. Using promoters, such as ZnO, enhances the performance of the catalysts. Our research investigated the adsorption behavior of H₂ and CO₂ on the Cu(111) and ZnO(10 $\bar{1}$ 0) surfaces using DFT-based quantum mechanical simulations. Our study revealed that H₂ chemisorbed dissociatively on Cu(111) and ZnO(10 $\bar{1}$ 0) with the binding energy of -0.331 eV and -2.02 eV, respectively. The atomic H preferred FCC site on Cu(111) and bound strongly with the O-atom of the ZnO lattice, indicating a strong hydrogen activation on these surfaces. However, CO₂ showed completely different behavior on these surfaces. CO₂ was physisorbed on Cu(111) with no structural changes, indicating poor CO₂ activation. CO₂ showed tridentate adsorption and chemisorbed on ZnO(10 $\bar{1}$ 0) with its bend configuration, forming a carbonate (-CO₃) species by combining CO₂ with the O-atom of the ZnO lattice. Similar observations regarding CO₂ adsorption on ZnO(10 $\bar{1}$ 0) have also been reported elsewhere^[2]. In conclusion, Cu(111) showed a better affinity for hydrogen, however ZnO can strongly activate both species. These findings prompt extensive research on optimizing the Cu-ZnO mixture composition for improved activation and stability of species and intermediates.

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Photocatalytic Degradation of Total Petroleum Hydrocarbon (TPH) Using Green Catalyst Under Visible Light

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Abstract

Petrochemical contamination from crude oil spills and drilling accidents is a leading cause of global pollution, posing a serious threat to all living species in the ecosystem¹. The potential of green nanomaterials in environmental and agricultural applications is gaining attention due to their biocompatibility, eco-friendliness, and cost-effectiveness². In this study, a green catalyst was synthesized using plant extract combined with transition and post-transition metals for the adsorption-assisted photodegradation of total petroleum hydrocarbons (TPH) in aqueous media. The synthesized composite was characterized by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), and Brunauer–Emmett–Teller (BET) analysis³. The photocatalytic activity was evaluated by monitoring the photodegradation of TPH under visible light, with gas chromatography-mass spectrometry (GC-MS) used to confirm TPH degradation. The significant degradation percentage demonstrates the effectiveness of the synthesized catalyst in addressing TPH contamination.

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Development of Chiral *cis*-2,5-Disubstituted Pyrrolidine Organocatalysts for Highly Enantioselective Michael Addition of Nitromethane to α,β -Unsaturated Aldehydes

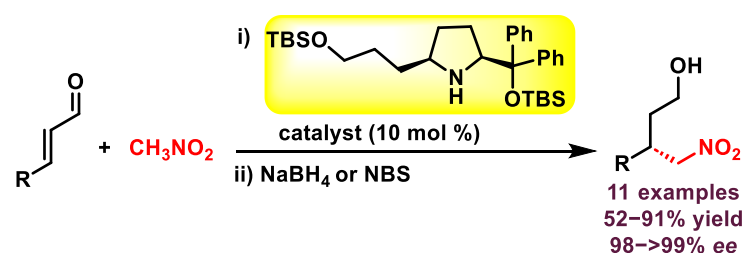
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Abstract

Single enantiomer drugs are preferred over racemic mixtures due to the homochiral nature of biological systems. Enantiopure β -substituted γ -aminobutyric acids (GABAs) exhibit more potency than their racemates. Hence, enantioselective synthesis of β -substituted GABA derivatives has garnered significant attention in medicinal chemistry and the pharmaceutical industry. The asymmetric Michael addition of nitromethane to α,β -unsaturated aldehydes is an attractive method for the synthesis of β -substituted GABA derivatives that can be catalyzed by various catalysts, including an engineered enzyme. In this work, we have developed the first synthesis of novel chiral *cis*-2,5-disubstituted pyrrolidine organocatalysts starting from the commercially available methyl L-pyroglutamate in six steps and demonstrated their application for the highly enantioselective Michael addition of nitromethane to α,β -unsaturated aldehydes. The enantioselectivity (>99% enantiomeric excess) obtained for the β -aryl-substituted γ -nitrobutyraldehydes, the key intermediates to access potentially useful β -substituted GABAergic drugs such as (R)-phenibut, (R)-baclofen and (S)-pregabalin, is unparalleled by other organocatalysts. The scalability of this methodology is showcased by a gram-scale synthesis.



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Theoretical Studies on the Mechanism of Water Splitting Driven CO₂ Reduction to CH₃OH/CH₄ on Metal Clusters

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Abstract

In the pursuit of sustainable energy and greenhouse gas emission reduction, the hydrogen evolution reaction (HER) and carbon dioxide reduction reaction (CO₂RR) have emerged as high priority research objectives. Of late, it has been shown that alkaline earth metal-based Mg (0) nanoparticles can be employed to split water to form H₂ and simultaneously in presence of CO₂ to reduce it to fuel feedstock chemicals like CH₃OH and ultimately to CH₄. Similarly, magnesium Mg (0) ribbon in granular sludge under anaerobic conditions can convert CO₂ to methane and upgrade biogas to biomethane under mild settings. This study employs Density Functional Theory (DFT) to investigate these reactions on Mg (0) clusters ranging from sub nanometer to nanometer length scale (Mg₂₂ and Mg₅₆), using water as the hydrogen source. Our findings reveal a low barrier pathway for CO₂RR using magnesium hydride, converting CO₂ to formic acid (HCOOH) and methanol (CH₃OH) which ensues after splitting of H₂O on surface Mg atoms forming Mg-H bonds. The subsequent reverse C-H activation reaction cleaves the C-O bond in methanol, yielding methane (CH₄) under ambient conditions without external energy inputs. These insights highlight the significant potential of magnesium-based clusters in green hydrogen production and CO₂ conversion.

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Investigation of the Impact of Oxygen Coverage on CeO₂-Supported Ag-Pd Alloy Catalysts for Hydrogen Production: A DFT Study

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Abstract

Formic acid is a promising liquid hydrogen carrier due to its renewable nature, low toxicity, and high hydrogen density.^{1,2} This study explores the impact of Ag alloying with Pd on interfacial sites and its influence on the selective production of H₂ from formic acid at ambient temperatures. Catalysts with a 0.5 PdAg-CeO₂ atomic ratio demonstrate superior H₂ selectivity (22%) and turnover frequency (TOF) of 98 h⁻¹ compared to Pd-CeO₂ (10% selectivity, 9 h⁻¹) at 298 K. The alloying of Ag induces electronic changes in Pd through charge transfer, wherein oxidised Pd reduces H₂ selectivity and promotes water formation. However, the specific role of oxygen and the mechanistic origin of the above catalytic performance remain uncertain. Density functional theory (DFT) calculations are being utilised to explore interfacial sites of Ag-Pd alloys on CeO₂ support, considering the effect of oxygen coverage. These factors are pivotal in modulating the adsorption behaviour, reaction pathways, and overall catalytic performance. The simulations will yield theoretical insights, guiding the synthesis of customised alloy nanoparticles. The ultimate objective is to advance sustainable hydrogen storage and transport, contributing to a cleaner and more energy-efficient future.

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A Mathematical Modeling Approach to Utilize CO₂ into Hydrogen and Electricity via Na-CO₂ Electrochemical System

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Abstract

The increasing CO₂ concentration, now at a record 419.3 ppm, is causing environmental problems, and current methods to reduce it are often inefficient and expensive.¹ Electrochemical conversion of CO₂ in aqueous electrolytes into a useful product has the potential to reduce the anthropogenic CO₂ concentration. CO₂ gas dissolves in aqueous solutions and produces HCO₃⁻, H⁺, and CO₃²⁻ and continuous purging of CO₂ lowers the pH, increasing H⁺ production.² Kim et al.³ have devised a hybrid Na-CO₂ system to utilize this to produce H⁺, hence CO₂ gas using a Na-metal as an anode, organic electrolyte, NASICON separator, aqueous electrolyte (CO₂ saturated NaOH solution) and Pt/C + IrO₂ coated carbon felt as the cathode. This system promises not only CO₂ utilization but also electricity and H₂ production.

This study develops a physics-based 2D multiphase transient mathematical model of the Na-CO₂ system using dilute solution theory, binary electrolyte theory, and laminar bubble flow in aqueous electrolyte. The local electrolyte current and potential distributions, species concentration distributions, and gas flow patterns are analyzed using this model. The model can be used to optimize geometric configurations, flow rates, CO₂ conversion, and chemical reactions and can potentially promote environmental sustainability and make the world greener.

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A CFD Study on CO₂ Desorption in an Aqueous MDEA Solution, Coupled Phase Transfer with Reaction Kinetics

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Abstract

CO₂ is one of the major constituents of greenhouse gases, that causes global warming. It is an acidic gas, causing oil piping corrosion and decreases the calorific value of the natural gas. It is important to separate the CO₂ from the gas stream[1]. The amine-based separation process involves two stages i.e., absorption followed by desorption. Extensive work has been done on the reaction kinetics of CO₂ with amines in the absorption process, whereas limited studies have been done on desorption rates of CO₂ from the loaded amines. Cadours et al.[2] experimentally investigated the desorption rates of CO₂ from the loaded aqueous MDEA solution. The regeneration of amine requires a large amount of energy and optimization of energy requirements in the desorption process is important [3]. To optimize the desorption process, we need to study phenomena such as two-phase gas-liquid counter-current flow, heat transfer, mass transfer coupled with the phase transfer, and flow in the porous zone, that affects the CO₂ desorption process. In this work, an Euler-Euler multiphase model based on an open source toolbox OpenFOAM is developed to study the effect of these phenomena on the CO₂ desorption process. The CFD multiphase model is coupled with the reaction kinetic model to simulate the reactive mass transfer. The developed model is validated against the experimental data given by Xu et al.[4].

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Chemical Depolymerization of Poly (lactic acid) into Methyl Lactate using Copper Supported Ceria as an Efficient and Reusable Catalyst

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Abstract

Chemical upcycling of plastic waste has attracted attention from all around the world because it offers a sustainable solution to the issue of plastic waste accumulation and helps create a circular plastic economy. One sustainable method of conserving resources and protecting the environment is by the chemical depolymerization and recycling of polylactic acid (PLA). The chemical depolymerization of PLA was investigated using Cu-CeO₂ as a catalyst, yielding methyl lactate (ML) as the product under relatively mild conditions, in order to achieve closed-loop recycling of PLA waste. In this work, we present an environmentally friendly and cost-effective approach for the methanolysis of polylactic acid. The PLA is completely depolymerized in the presence of Cu-CeO₂ catalyst at 140 °C for 8 h. In order to get the best catalytic activity and product selectivity, the reaction condition was optimized. ¹H NMR spectroscopy is used to support the detailed depolymerization mechanism. Experiments on a larger scale were also carried out to demonstrate the synthetic utility of the designed reaction protocols. The effectiveness and sustainability of the designed protocols were demonstrated by the evaluation of the green metrics parameters, paving the way for the industrial upscaling of plastic depolymerization. This study offers a sustainable, low chemical input and environmentally friendly method for chemically recycling these plastics.

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Efficient Electron Injection into Graphullerene Enables Reversible NaC₂ Sodium Storage

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Abstract

Sodium-ion batteries are emerging as promising alternatives to conventional lithium-based technology, offering solutions to challenges in large-scale grid storage.¹ However, weak thermodynamic interactions and irreversible structural changes leads to slow kinetics of (de)intercalation for Na-ions that hampers the Na storage capacity of conventional graphite-based anodes.² Herein, we present a computational design that explores the potential of graphullerene,³ a 2D framework with interconnected fullerene moieties, for the reversible storage of Na-ions. A unique aspect of this design is the utilization of fullerene moieties' electron acceptance capacity for large-scale ion storage. To implement this, the electrochemical traits of graphullerene sheet is assessed through DFT and AIMD-based computational approaches, employing suitable DFAs and the recently developed non-local variant of many-body dispersion (MBDNL) schemes. Our study demonstrates that the high electron injection capacity of sodium into graphullerene supports a high Na-to-C stoichiometry (NaC₂). Additionally, a multilayered arrangement of Na ions enables superionic diffusion on the graphullerene surface via a cooperative mechanism.⁴ The important outcome of this study is that raising the electron injection limit offers a promising strategy to transform carbon-based anodes into suitable candidates for reversible Na-ion storage, without relying on artificial defect introduction or doping.

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Theoretical Insights and Catalyst Design for Bio-Renewable Substrate Transformation

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Abstract

Theoretical calculations play a pivotal role in unraveling complex surface phenomena and reaction mechanisms, providing crucial insights that guide rational design of efficient and selective catalysts for bio-renewable substrate transformations. To understand the mechanism involved in reductive amination of 5-HMF, we used both Density Functional Theory (DFT) and *ab-initio* Micro-kinetic Modelling (MKM) and suggested bimetallic catalysts to mitigate nitrogen-induced deactivation. In another work, structure-dependent activity and selectivity in furfural acetalization were investigated using both DFT simulations and experiments on Pd nanostructures. Pd cubes were found to be most active with methanol as solvent. Here, hydrogen bonding networks between solvent molecules and adsorbates reduced activation barriers and stabilized the transition states. To understand the metal/solvent effect further in maleic acid to succinic acid hydrogenation, we used both DFT and *ab-initio* Molecular Dynamic (AIMD) simulations. Additionally, to streamline catalyst screening, machine learning along with DFT simulations were used to predict the descriptor binding energies on Cu-based bimetallics where xGBR model gave the best results. Further, *ab-initio* MKM was used to predict the turnover frequencies over these predicted bimetallics. This integrated approach, combining DFT, MKM, and ML, offers an effective strategy for designing metal and bimetallic catalysts in catalytic transformation of bio-renewable substrates.

Computational Insights into the Structural and Opto-Electronic Properties of BiCuP₂S₆ and BiCuP₂Se₆ Metal Chalcophosphates

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Abstract

Metal chalcophosphates, with the formula M₂P₂Q₆ (where M denotes transition metals and Q represents chalcogens), are noteworthy within the van der Waals materials family. However, there is limited systematic research on how their fundamental structures change with different metal cations, largely due to challenges in incorporating these cations into the octahedral sites of the M₂P₂Q₆ framework^[1-5]. Our study provides a detailed computational characterization of BiCuP₂S₆ and BiCuP₂Se₆, both of which are dynamically stable materials. Using density functional theory (DFT) and other advanced computational methods, we investigate their structural, opto-electronic, catalytic, and excitonic properties. Our analysis reveals that these compounds display distinct structural motifs influenced by their chalcogen components. Electronic band structure and density of states calculations, conducted with various functionals, show significant differences in their band gaps. These findings offer valuable insights into the potential applications of BiCuP₂S₆ and BiCuP₂Se₆ in solid-state devices, highlighting how chalcogen substitution and metal alloying can modulate their opto-electronic and catalytic properties. This computational study sets the stage for future experimental research and the development of materials with tailored functionalities.

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Li/Na/K-Al-Sc Cluster Compositional Space for Electrochemical Hydrogen Evolution and Nitrogen Reduction Reaction

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Abstract

The development of efficient catalysts for sustainable energy conversion, particularly in the Hydrogen Evolution Reaction (HER) and Nitrogen reduction reaction (NRR), is a critical challenge for addressing global energy demands.¹ Atomically precise metal nanoclusters have emerged as functional materials for addressing various challenges in diverse electrocatalytic applications.² Multi-atom catalysts with atomic precision are frontier in heterogeneous catalysis with synergistic effect while maintaining high atomic utilization efficiency and good selectivity for efficient electrochemical H₂ and NH₃ production which is not only fundamentally important but also economically vital.³ This study investigates the magic-sized metal clusters based on (Li/Na/K)-Al-Sc compositional space in enhancing catalytic activity, with a focus on tailoring geometric and electronic properties using density functional theory (DFT). An important outcome of this study is the elucidation of the precise scandium concentration in (AM)Al_{13-x}Sc_x (AM=Li, Na, K) clusters for selective HER and NRR. In addition, we systematically explore the mechanistic insights into electrocatalytic H₂O-to-H₂ and N₂-to-NH₃ conversion.⁴ Overall, our findings shows that high entropy magic-size clusters with precise compositional engineering strategy leads to selective HER and NRR with improved efficiency.

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Role of the Cu^+/Cu^0 , Acidic-Basic Sites, and the Oxygen Vacancy for the Hydrodeoxygenation of the Lignin-Derived Compounds

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Abstract

The world's energy demand rapidly increases due to population growth and industrial and economic development. Fossil fuels like oil, coal, and natural gas currently meet most energy demands but are non-renewable and may soon be depleted. Renewable sources such as solar, wind, and biomass are crucial for meeting future energy needs and reducing carbon emissions. Among all the renewable energy sources, biomass has a unique advantage. Biomass, producing around 170 billion metric tons annually, contains cellulose, hemicellulose, and lignin. Lignin, the second most abundant component after cellulose, is a renewable source of aromatic feedstock available globally. Despite its potential, lignin remains underutilized compared to cellulose and hemicellulose. In this aspect, we have developed a Cu/MgAlO_4 (CMA1.5) catalyst derived from the CuMgAl-LDH (CMA-LDH) precursor via topological transformation for the catalytic hydrodeoxygenation of the lignin-derived compound to produce value-added chemicals. A comprehensive analysis of the as-synthesized catalysts has been conducted using various characterization techniques, confirming their intriguing properties, and promising activity for the hydrodeoxygenation of vanillin to the 2-methyl-4-methoxy phenol (MMP). Furthermore, multiple control reactions helped to clarify the reaction mechanism, and substrate scope tests demonstrated the reaction's wide applicability. This work highlights a greener, sustainable method for hydrodeoxygenation of biomass-derived compounds.

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Unveiling Mechanistic Descriptors for the Acid-Catalyzed Dehydration Reaction: A Strategic Approach to Solvent Design

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Abstract

Selective catalytic upgrading of biomass-derived feedstocks to fuels and chemicals is considered difficult owing to the complexity of the constituent's chemical structure and reaction environment.¹ A firmly established strategy for the conversion of biomass-derived lactone molecules to useful chemicals involves the removal of oxygen-based functionalities via acid-catalyzed dehydrations.² In these reactions, the choice of solvent is as crucial as the choice of catalyst, significantly influencing the production of biorenewable chemicals.³ Mevalonolactone (MVL), featuring a cyclic ester and hydroxyl groups, is an ideal biomass-derived platform chemical for studying acid-catalyzed reactions in solvents.⁴ To design effective solvents for MVL dehydration, a molecular-level reactivity descriptor was examined in organic solvent tetrahydrofuran (THF), water, and their mixtures. This descriptor acts as a mechanistic switch in the MVL dehydration reaction. Substituting water with THF resulted in a significant reduction in the reaction's free energy barrier, decreasing from 108 kJ/mol to 82 kJ/mol, as revealed by ab initio molecular dynamics (AIMD) and metadynamics simulations. The mechanistic descriptor was measured as the coordination number of water molecules that strongly interact with the cyclic ester group of MVL at various THF/water ratios. This descriptor demonstrated a strong correlation with both experimentally observed MVL conversion and theoretically calculated free energy barriers for the dehydration reaction, providing important insights for designing optimal solvents.

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Neural Networks Enable in-Depth Insights into Coverage and Cation Effects in Electrocatalysis

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Abstract

A realistic modeling of (electro)catalytic interfaces poses considerable challenges due to the inherent complexity of the catalyst surface and the dynamic reaction environment present under operating conditions.¹ In this work, I will present our work on using neural networks to tackle the complexities of (electro)catalytic interfaces. In particular, I will discuss two examples involving the use of message-passing neural networks² to study cation and adsorbate coverage effects. In the first example, we train neural network interatomic potentials using active learning workflows to study the impact of alkali metal cations on the structure of electrified Au interfaces. We find several properties including water coverage, orientational distributions and vibrational density of states of water molecules, ion solvation, and double layer capacitance to be sensitive to the cation identity and surface charge density. In the second example, we use high-throughput simulation pipelines and neural network models to estimate coverage-dependent CO adsorption energies on low and high index facets of Cu, and co-adsorption of species on Rh surfaces.³ Our findings highlight the promise of using neural network accelerated atomistic simulations towards realistic modeling of (electro)catalytic interfaces.

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A Novel Mechano-synthesized Zeolitic Tetrazolate Framework for High-Performance Triboelectric Nanogenerator and Self-Powered Selective Neurochemical Detection

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Abstract

Designing a high-performing triboelectric novel material with eco-friendly, rapid, cost-effective synthesis is the future of material research in triboelectric nanogenerators (TENG). We report a mechanochemical ball mill synthesis of a Zeolitic Tetrazolate Framework (ZTF-8) which is isostructural with the well-known zeolitic imidazolate framework ZIF-8. ZTF-8 is extremely stable in water, 0.1 M aqueous acid and base solutions for 75 days and boiling water for 7 days. Three-Dimensional Digital Microscopy, Atomic Force Microscopy, Kelvin probe force microscopy and Molecular Electrostatic Surface Potential computational analysis reveals the high roughness profile and benchmarking surface potential in the ZTF-8 film. The unique structure, exceptional acid/base stability, good dielectric property, high roughness profile combined with extreme surface potential of ZTF-8 makes it as a suitable candidate as a polymer free triboelectric positive material in TENG with outstanding performance (power density of 720 mW /m²). In addition, the efficiency of ZTF-TENG was utilized as a self-powered device for selective dopamine (DA) sensor with good sensitivity, wide range linearity, and excellent limit of detection. This report is extremely distinct and stand-out due to the fact that the developed TENG device's positive layer contains no polymer participation but still provides excellent performance and selective neurochemical sensing behavior.

Metal-Free Impregnated Carbon for Efficient Toxic Gas Removal: A Sustainable Approach for Environmental Cleanup

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Abstract

Sulfur dioxide (SO₂) emissions pose a significant threat to the environment and human health, necessitating efficient methods for their removal from industrial effluents and exhaust gases. In this context, the development of efficient and eco-friendly gas removal technologies is of paramount importance. This study investigates the synthesis, characterization, and application of metal-free impregnated carbon materials for the removal of noxious gas SO₂ from air and industrial effluents. In this study, five different ionic liquid is impregnated with activated carbon by incipient wetness technique. Furthermore, the synthesized metal-free ionic liquid impregnated carbon materials were comprehensively characterized using PXRD, SEM, TGA, FTIR, & BET. Adsorption experiments were conducted at ambient temperature, pressure and at various RH, loadings and gas concentrations, to evaluate the materials' performance. Out of 5 ionic liquids, it was observed that 5%1-dodecyl-3-methylimidazolium iodide (5%ID3MIMI) showed the best removal efficiency against SO₂ for the concentration of 1500 pm at RH (65±5) %. The NMR, UV-Visible, SCXRD, Raman, CHNS, and XPS analysis provides insight into mechanism and their structural and chemical properties. This study not only contributes to the development of effective SO₂ removal technologies but also emphasizes the importance of using non-metallic impregnating agents, ensuring environmentally friendly gas removal processes.

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Effect of Synthesis Parameters on the Optoelectronic Properties and Photoelectrochemical Performance of BiFeO₃ Thin Films

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Abstract

Bismuth ferrite (BFO) is a cost-effective, relatively earth-abundant multiferroic semiconductor with tunable optoelectronic properties capable of absorbing visible light ($1 \leq 600$ nm)^{1,2}. Due to its phase-dependent ferroelectric behavior, it is proposed to enhance the charge generation yield, which can potentially enhance the efficiency of a photocatalytic reaction³. Despite these promising prospects and having appropriate thermodynamic driving energy, utilization of BFO for water-splitting reactions and/or biomass oxidation is limited. It may be linked partly to lack of comprehensive understanding of the defect chemistry involved and the resulting charge separation/transport properties. Our work aims to understand the effect of synthesis parameters and investigate photoelectrochemical water oxidation reaction. In this direction, the structural and optoelectronic properties of BFO are systematically controlled by tuning the synthesis parameters such as annealing atmosphere and precursor ratio. Annealing in an inert atmosphere improved the crystallinity of BFO thin films, consequently increasing the photocurrent density by ~ 1.6 times compared to BFO prepared by annealing in ambient air. Changes in the inherent defects formed were rationally correlated with the photoelectrochemical water splitting performance. Results highlight the importance of elucidating the fundamental synthesis-structure-property correlation to improve the photocatalytic performance of BFO.

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Distinction of Plasmonic Intrananoparticle and Internanoparticle Molecular Reaction Rates Based on Phase Transition at the Three-Phase Contact Line of an Evaporating Sessile Droplet

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Abstract

Natural ring stain formation upon evaporation of a sessile droplet with dispersed particles continues to attract great scientific attention. We observed the deposition process is akin to a phase transition¹ with particles depositing at the contact line in a short span of time and well before the complete drying of the droplet. Molecular reactions on the surface of plasmonic nanoparticle (intrananoparticle) and in between nanoparticles (internanoparticle) may differ in kinetics, dynamics and product selectivity. We report that the difficulty in distinguishing the kinetics in a dispersion medium could be overcome by probing the reactions at the three-phase contact line (TPCL) of an evaporating sessile droplet using surface enhanced Raman spectroscopy (SERS).² Thus, when an evaporating aqueous droplet on glass, containing 4-aminothiophenol (4-ATP)-stabilized Ag nanoparticles, was monitored by SERS at the TPCL, dimerization into 4,4'-dimercaptoazobenzene followed two steps, each preceded by the loss of H-bonded water accordingly. Based on the results, we assigned the first step with higher relative kinetic rate (~3 times) to be intra-nanoparticle and the second one as inter-nanoparticle reactions. In D₂O medium, the ratio of the rates was ~1.8. The observed vibrational signatures of the losses of water molecules before reactions and product formations were accounted for using density functional theoretical calculations.

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Covalent Organic Frameworks as Nano-Reservoir for Room Temperature RNA Storage

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Abstract

The emerging role of Ribonucleic acids (RNAs) as therapeutics is alluring.¹ However, RNAs are extremely labile under ambient conditions and typically need to be stored in cryogenic conditions ($-20\text{ }^{\circ}\text{C}$ to $-80\text{ }^{\circ}\text{C}$).² Hence, storage, stabilization, and transportation of RNA under ambient conditions have been an arduous task and remain an unsolved problem. In this work,³ a guanidinium-based ionic covalent organic framework (COF), TTG_{Cl} with nanotubular morphology, was synthesized and used as nano-reservoirs for room-temperature storage of RNA. To understand the role of the nanotubular morphology and chemical nature of TTG_{Cl} in stabilizing the RNA structure and for comparison purposes, a neutral COF, TMT-TT, is synthesized and studied. Further, density functional theory (DFT) studies confirmed non-covalent interaction between the COFs and the RNA nucleobases, facilitating reversible storage of RNA. RNA loaded in COFs was found to be resistant to enzymatic degradation when treated with RNase. Gel electrophoresis and sequencing confirmed the structural integrity of the recovered RNAs and their further processability.

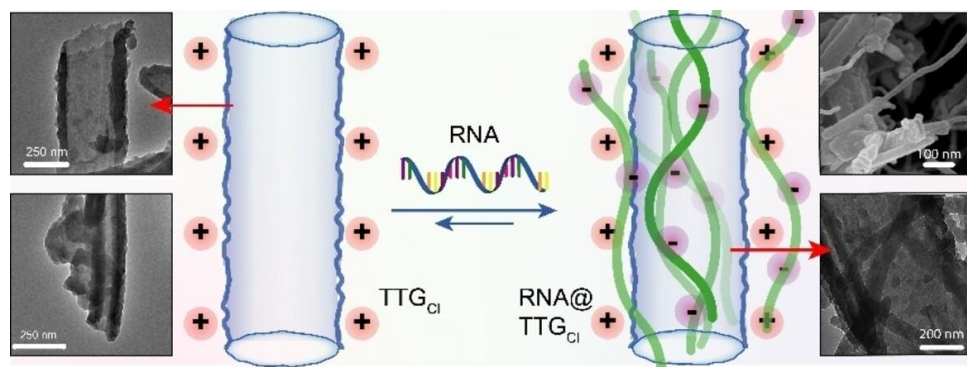


Figure 1: Schematic representation of storage of RNA in TTG_{Cl} COF.

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Heterogeneous Catalytic Cyclopropanation of Structurally Diverse Alkenes in Aqueous Medium

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Abstract

Recent advances in sustainable chemical synthesis highlight the use of bio-catalysts, such as metal porphyrins in enzymes, for efficient and selective cyclopropanation. These natural catalysts excel in regio- and stereoselectivity, but their practical application is hindered by challenges in enzyme stability and synthesis. Consequently, enzyme mimics have been explored but face issues with catalytic activity, stability, and recovery in aqueous solutions.

To address these limitations, our research focuses on developing a heterogeneous catalyst for cyclopropanation in water by incorporating metal porphyrins into confined spaces like silica core-shell structures. Specifically, we examined functionalized SBA15 materials, which provide a stable, hydrophobic environment for metal porphyrins. Using Hemin as the catalytic center, we achieved improved catalyst longevity and recyclability. The encapsulated metal-porphyrins demonstrated easy recovery and regeneration from the reaction mixture, enhancing their practical application in green chemistry which are the advantages of the material over to bulk or solution state Hemin.

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Green Synthesis of SO₃H-Functionalized ZnS/Biochar Nanocatalyst: Enhanced Glycerol Acetalization and Reusability in Methylene Blue Dye Adsorption

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Abstract

In this work, we have reported the successful synthesis of an acid-functionalized ZnS/Biochar (ZBC-SO₃H) nanocatalyst through a co-precipitation method utilizing *Camellia sinensis* leaf extract. The acidic nature is the essential component for the acetalization of glycerol with acetone, and the solketal yield is determined mainly by the surface acid density of catalysts [1]. Solketal is a very valued glycerol ketal because of its prospective uses as a green solvent, and plasticizer in the polymer sector [2], and suspending and solubilizing chemicals in biodegradable units for the regulated emission of medicinally active compounds. The ZBC-SO₃H nanocatalyst was employed for the microwave-assisted acetalization reaction of glycerol with acetone for selective solketal synthesis (biofuel derivative). The catalyst was reusable up to 6 reaction runs in the solketal synthesis, which remarks the high stability of the ZBC-SO₃H. Further, the reusability of the ZBC-SO₃H (remaining catalyst after 6 runs) was examined in the adsorption of methylene blue (MB) dye [3]. Additionally, the large surface area (326.21 m²/g) and high total acid density (1.98 mmol/g) favor the excellent catalytic activity of the ZBC-SO₃H nanocatalyst.

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Synthesis of Conducting Polymer-Chitosan/Metal Oxide-based Nanocomposites for Advanced Applications

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Abstract

The development of nanocomposites presents a transformative approach to address wide array of global challenges. We employed an advanced *in situ* oxidative polymerization method to synthesize innovative Polyaniline-Chitosan-ZnO nanocomposites. These NCs were characterized using techniques like FTIR, UV-Vis spectroscopy, SEM, SEM-EDX, and XRD to gain insights into their structural and morphological properties. The multifunctional nature of these NCs was demonstrated through their exceptional anti-corrosive, dye adsorption, and antibacterial properties. Specifically, our findings revealed that the nanocomposites exhibited an impressive 85% anticorrosion efficiency on mild steel, as determined by the weight loss method. Moreover, they displayed remarkable capabilities in adsorbing Methylene Blue dye, achieving an outstanding 89.62% dye removal from aqueous solutions within just 5 h under sunlight, thus showcasing their potential for efficient water purification applications. Furthermore, antibacterial properties of these nanocomposites against *Staphylococcus aureus* using spot assay analysis unveiled a dose-dependent inhibition effect and significant antibacterial activity, underscoring their potential for antimicrobial applications. These findings not only emphasize the versatility of Polyaniline-Chitosan-ZnO NCs but also position them as highly promising candidates for addressing multifaceted challenges in corrosion protection, environmental remediation, and antimicrobial applications.

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Novel Strategy to Design Functional Ceramic Oxides by Temperature Controlled Topotactic Reaction at the Interface of Composite Phases

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Abstract

LaFeO₃ exhibits antiferromagnetic ordering at 740 K. Interestingly, although LaFe_{0.5}Mn_{0.5}O₃ exhibit long-range ferromagnetic for M=Cr at 120 K and antiferromagnetic ordering for M=Co & Ni at 370 and 100 K respectively, LaFe_{0.5}Mn_{0.5}O₃ lacks of such ordering. This makes LaFe_{0.5}Mn_{0.5}O₃ a central focus to address: (i) physics behind the lack of spin ordering and (ii) how to achieve spin ordering in a ceramic sample. For the first time, we observe the long-range magnetic ordering in ceramic powder by the entanglement of cation ordering through temperature controlled interfacial topotactic reaction between La_{0.45}Ca_{0.55}MnO₃ and LaFeO₃ in nanocomposite form. The ferromagnetic T_C of 225 K [1] for powder sample is comparable to the 1:1 superlattice stacking of LaFeO₃-LnMnO₃ of T_C=230 K [2]. The interfacial cation ordering is highly sensitive to the processing temperature and hence the magnetism. The present study demonstrates a new strategy to design functional material through temperature controlled topotactic interfacial reaction. This has been substantiated by the synthesis and magnetization of well-known double perovskite La₂MnCoO₆ [3] starting from LaMnO₃ and LaCoO₃ in the composite form. This approach may possibly be utilized to design new functional materials from multicomponent composite system.

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Development and Assessment of Novel Lubricity Enhancers Additives for Ultra Low-Sulfur Diesel Fuel

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Abstract

Ultra Low-sulfur diesel fuel (ULSD) is necessary to meet stringent regulations, achieved through the extreme hydrodesulfurization of conventional diesel fuel. Extreme hydrodesulfurization reduced the lubricating property of diesel fuel. Therefore, ULSD fuel requires additives or compounds that can enhance the lubricity of diesel fuel. This work synthesizes a heteroatomic-containing additive as a lubricity-enhancing additive of ULSD fuel. The additives were synthesized by the reaction between 3,5-di-tertbutyl-4-hydroxybenzaldehyde and 3-amino-1,2,4-triazole. The synthesized additives were analyzed using infrared (FT-IR) and nuclear magnetic resonance (NMR) spectroscopy. The lubricity of neat ULSD fuel and ULSD with different concentration of additives is measured using a high-frequency reciprocating rig (HFRR) according to the ASTM D6079 method. The effect of additives on the lubricity of low-sulfur diesel fuel was evaluated in terms of average wear scar diameter (AWS) and average friction coefficient. The result shows that ULSD fuel exhibits an AWS of 413 μm and an average friction coefficient of .202. Adding 0.5 to 1.5% of additives to the ULSD fuel significantly reduced the AWS and average friction coefficient. However, the AWS and the average friction coefficient show a 31.96 % and 24.2 % reduction, respectively, with the addition of a 1.5% additive concentration.

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A Comparative Analysis On Supercapacitive Behaviour Of Bimetallic Ni-Co-Layered Double Hydroxides With Monometallic Ni/Co Layered Double Hydroxides

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Abstract

Nanostructured metal hydroxides and oxides are recognized by their unique redox-active behaviour, which make them ideal materials for advanced energy storage.^[1] Among them, Ni and Co based nanostructures have particularly attracted significant attention due to their high theoretical capacitance^[2,3] and taking advantage of their synergistic effect can be even more promising. Herein, bimetallic Ni-Co based layered double hydroxide (LDH) and their corresponding pure hydroxides (Ni-LDH and Co-LDH) were synthesized via homogeneous precipitation method using similar synthetic conditions. The synthesized LDH phases were characterized using various techniques. The distinct morphologies of Ni-LDH, Co-LDH and Ni-Co-LDH as revealed from FE-SEM are nanosheets, nanorods and dahlia-like nanopetals, respectively. The electrochemical characterization demonstrates that Ni-Co LDH achieves a specific capacitance of 1434.5 F g⁻¹ at 10 mV s⁻¹, which shows about 6 fold enhancement as compared to pure Co-LDH (239.3 F g⁻¹) and a 156 F g⁻¹ enhancement as compared to Ni-LDH (1278.5 F g⁻¹). The superior electrochemical behaviour of Ni-Co-LDH can be attributed to synergistic effect of presence of both Ni and Co and its higher electrical conductivity.^[4,5] The excellent electrochemical performance of Ni-Co-LDH has a great potential for next-generation energy storage devices.

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Ionic Liquid-Supported D-A Type Conjugated Polymeric Material Based on Vat Dye Congo Red as a Photosensitizer for DSSCs

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Abstract

Vat dyes are the greatest candidates for organic dyes that exhibit redox activities.¹ Vat dye based polymers become effective sensitizer material for dye-sensitized solar cells (DSSCs) because of their higher absorption coefficient and redox properties by reducing the polymeric film thickness.²⁻³ Herein, an ionic liquid (IL) supported D-A type conjugated polyimide sensitizer was synthesized derived from vat dye Congo red and pyromellitic dianhydride (PMDA) via condensation polymerization technique. This polymeric material is doped with BF₃ and supported with a minimal quantity of IL for better conductivity results and interface creation. The synthesized polyimide exhibited favorable oxidoreduction properties with a narrow band gap of 1.96 eV, and good electrical conductivity (>10⁻⁴ S/cm), indicating its semiconducting nature. The photovoltaic characteristics of the fabricated electrodes and DSSC were assessed, yielding J_{sc} = 0.2324 mAcm⁻², FF = 0.6906, and V_{oc} = 0.2380 V., resulting in a power conversion efficiency (PCE) of 0.04%. The film-forming properties of the polymeric sensitizer may mitigate electron passivation within the cell, highlighting its potential applicability in DSSC technology.

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Development of 808 nm NIR Responsive Self-Sensitized Upconversion Nanocrystal

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Abstract

In recent times, 980 nm-responsive NIR-upconverting crystalline nanoparticles have found extensive application in the field of biomedicine. However, due to the strong water absorption profile of 980 nm excitation, the concerned upconverting nanoparticle (UCNP) suffer from heating effect. Also, Nd³⁺ sensitized 808 nm excitation had weak intensity and thus in order to improve UCL efficiency, core-shell structured UCNPs were designed, in which activator and Nd³⁺ were doped in inner core and outer shell, respectively, in order to minimize the cross relaxation. In this work, a pathway for developing 808 nm-responsive core UCNP with intense and diversified emission profile is described. Apart from synthesizing the UCNP with enhanced emission profile, a thorough characterization of the crystalline structure at the local level has been proposed. Detailed mechanism behind the intensification of the emission profile is to be investigated using exhaustive synchrotron X-ray diffraction study. Finally, the superior photodynamic activity of the proposed UCNP with enhanced emission profile is to be validated through few basic applications. The proposed work is expected to gather fundamental knowledge on crystal engineering-based nanotechnology.

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The Effect of Dopant Concentration on the Upconversion Process of $\text{NaYF}_4:\text{Yb}^{3+}, \text{Er}^{3+}$ Nanocrystal

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Abstract

Lanthanide doped upconverting materials in the recent times have attracted great attention due to their unique optical properties such as large anti-stokes shift, sharp-band emission, long emission lifetime, superior photo stability and near-infrared excitation. These materials have potential applications in biological imaging, medical diagnosis, color displays, temperature sensing and so on. The dopant concentration of lanthanide ions in photon upconversion nanoparticles (UCNPs) remain one of the key point to enhance the upconversion luminescence intensity and, therefore, their application developments. Here, we have analyzed the effect of Yb^{3+} dopant concentration on $\text{NaYF}_4:\text{Yb}^{3+}, \text{Er}^{3+}$ nanoparticle for the visible upconversion phenomena by employing two different synthetic route i.e thermal decomposition and coprecipitation. The high doping of the sensitizer Yb^{3+} will accelerate the population of both green and red emitting energy levels, but cause significant concentration quenching in the green emission and little quenching in red emission. Further, we have tried to do in depth analysis of the crystal structure using different characterization technique like TEM, FESEM, synchrotron based SXRD and rietveld refinement study for the phase purity. This work offers in-depth insight into the UC mechanism of Yb^{3+} doped $\text{NaYF}_4:\text{Yb}^{3+}, \text{Er}^{3+}$ and engineering of novel luminescent materials with distinguished properties.

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Upconversion Properties and Optical Temperature Sensing of Yttrium Tungstate-based Host Crystals

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Abstract

The attraction of photon upconversion through the use of lanthanide-doped materials involves generation of photons at shorter wavelengths than the excitation wavelength after laser stimulation. Besides their extensive use in the field of bioimaging, drug delivery and sensors, temperature sensing based on the fluorescence intensity ratio (FIR) that suffers with low sensitivity still needs host crystal with strong upconversion luminescence (UCL) intensity. Here a series of $\text{Y}_2\text{WO}_6:\text{Er}^{3+}/\text{Yb}^{3+}$ crystals were synthesized via high temperature solid state method. For enhancing the UCL intensity, the crystal engineering route has been adopted by introducing a non-lanthanide ion (Li^+) in different mol % inside the host lattice. The respective UCL intensities as well as the absolute sensitivity got enhanced. An in-depth structural analysis has been done by using the synchrotron X-ray diffraction (SXRD) experiments to trace the structural changes inside the crystal lattice after incorporation of Li^+ , responsible for the above enhancement. As there are no major changes has been noticed in terms of structural and morphological analysis, we headed for an atomic level study by calculating the lattice strain from the SXRD data using Williamson-Hall method. Interestingly, at the highest value of strain, the local disorder is utmost with maximum UCL intensity and absolute sensitivity.

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Value Addition of Lemongrass Oil through Synthetic Transformation of its Major Constituent

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Abstract

The Himalayan region is a rich source of high value aromatic crops. Under Aroma Mission of CSIR, the Institute is working on development of improved varieties, agrotechnology, processing and value addition of Himalayan aromatic crops for improving rural economy of this region. In current work a comprehensive approach for the transformation of essential oil into value added compounds has been developed. The study focuses on the efficient synthesis of β -ionones from lemon grass essential oil a rich source of citral, into high-value aroma compounds like β -ionones. β -ionones also serves as precursor for vitamin A and key intermediates in the fragrance industry. Our main goal is to identify reaction conditions under which the lemon grass oil can be converted into value added product with single ionone isomer. Further, we are targeting the derivatisation of pure isomer through advance synthetic methodologies. These advance methodologies will enable the development of novel compounds with potential applications in both pharmaceuticals and fragrance industries.



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Co(III)-catalysed Site-selective C8-Allylation and Vinylation of Isoquinolones with Allyl Acetate and Vinyl Acetate

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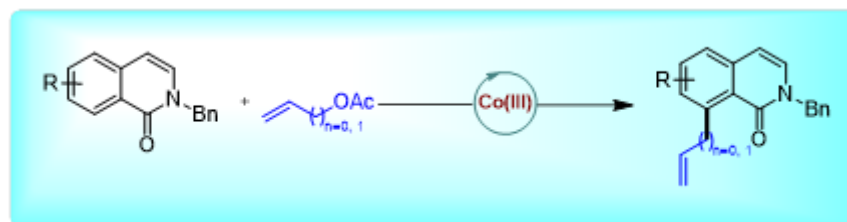
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Abstract

Isoquinolones are important building blocks for synthesizing various natural products and biologically important molecules.^{1,2} Herein, we have reported Co(III)-catalysed site-selective allylation and vinylation at C8 position of isoquinolones by using allyl acetate and vinyl acetates as an effective surrogates of the allyl and vinyl groups.³ The oxo group of isoquinolone has been utilised as a native directing group. A plausible catalytic cycle has been delineated based on the preliminary mechanistic experiments. The synthetic utility of the developed methodology was showcased by scale-up synthesis and transformation of the products into useful building blocks.



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MLCT-Driven Solar Fuel Production using a Fe-Terpyridine-Based Soft Coordination Polymer Gel

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Abstract

Coordination polymers (CPs) are recognized for their robust structures and strong covalent interactions, making them valuable in storage, separation, optoelectronics, and catalysis. However, their poor solution processability limits their applications and efficiency. To address this, coordination-driven supramolecular polymers (CSPs) or coordination polymer gels (CPGs) offer a promising alternative due to their solution processability, particularly in catalysis. While these systems have been studied as soft metal-organic materials for optoelectronics, their application as photocatalysts with controlled nanostructures remains under explored. In this study, a low molecular weight gelator (LMWG) derived from terpyridine (TPY)-linked naphthalenediimide (NDI) (TPY-NDI) was synthesized and used in metallo-supramolecular polymerization. The self-assembly featuring Fe(II) with TPY-NDI coordination with different stoichiometry and solvents results in different nanostructures with different morphologies. The different nanostructures were employed for CO₂ reduction under visible light and the 1D nanofibrous metallo-supramolecular polymer showed the highest rate and selectivity for CH₄ production, achieving 2.75 mmol g⁻¹ h⁻¹ with >96% selectivity. In-situ DRIFT spectroscopy and DFT calculations suggested a plausible mechanism for CO₂ reduction to CH₄.

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Lignocellulosic Biomass Conversion to Furans-Based High Value Molecules

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Abstract

The plentiful amount of agro-waste is considered as a promising candidate for production of bio-based high value compounds. In this context, 5-hydroxymethylfurfural (5-HMF) and furfural emerged as pivotal platform chemicals for biofuel, biopolymers and other high value chemicals production.¹ Considering the high need for agro-waste valorization, our research group has been consistently working on biomass conversion into 5-HMF and furfural, and its further functionalization into value-added compounds.² In continuation to our previous work, herein, we developed a greener, highly selective, scalable, and economical approach for the conversion of de-oiled lemongrass waste, sugarcane bagasse, rice straw, and corn cob into 5-HMF and furfural with 51-64 and 48-61 mol% yields respectively under hydrothermal reactor system. Under this study, the combined effects of both organic and inorganic acids and other reactions parameters were thoroughly examined. Overall, the developed method offers a more environmentally friendly and product specific approach for converting lignocellulosic biomass into furanic compounds, and avoiding the use of expensive metal catalysts.

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One Pot Synthesis of Worm-Hole Like Tunable Amine Functionalized Silica Catalyst for Carbon Dioxide Utilization into Cyclic Carbonates

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Abstract

A silica catalyst with characteristic features of broad pore size distribution, large pore volume and tunable Lewis acidic and basic sites was synthesized by a one-step greener co-condensation synthesis method analogous to SBA-15 synthesis. Tunability of the above catalytic key features are proved by N₂, CO₂ and NH₃ absorption and desorption experiments. The catalyst achieves 90% conversion of styrene oxide (SO) with nearly complete selectivity towards styrene carbonate (SC) in just 7 hours under solvent free condition at a temperature of 120 °C with co-catalyst tetrabutylammonium bromide (TBAB). Moreover, the catalyst demonstrates versatility with various epoxide substrates, providing valuable insights into this 100% atom economic cycloaddition reaction under ambient pressure conditions involving carbon dioxide. A mechanistic understanding of the catalytic conversion was investigated with the help of in-situ FTIR/ DRIFT studies.

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Eco-Friendly Fabrication of WO₃ Nano dices for Efficient Ciprofloxacin Degradation

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Abstract

Contaminated water poses serious risks to human health and the environment, with traditional treatment methods often falling short. Photocatalysis, however, offers a promising solution by breaking down organic pollutants using light.^[1] Recent advancements focus on nanostructured photocatalysts, especially those activated by visible light, due to their efficient sunlight utilization and low energy requirements.^[2]

Enhancing these photocatalysts' performance involves strategies like phase control, surface sensitization, and doping.^[3] One challenge is the high recombination rate of photo-generated electron-hole pairs, which can be addressed by integrating carbonaceous materials, such as activated carbon (AC). AC's high surface area and pore structure enable effective adsorption of pollutants and facilitate reactions that reduce electron-hole recombination.^[4]

We are currently investigating the development of composites with metal oxides using activated carbon (AC). The inclusion of carbonaceous materials facilitates the reaction between adsorbed oxygen and photogenerated electrons, effectively reducing the recombination of electron-hole pairs. This combination promotes efficient adsorption and photocatalytic oxidation due to AC's functional groups, which help prevent recombination as well as release of toxic by-products.

In summary, integrating AC with metal oxides shows significant potential for creating efficient, sustainable photocatalysts for water treatment, addressing both environmental and economic concerns.

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Tailoring Zeolites for Enhanced Plastic Waste Upcycling Efficiency

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Abstract

The growing concerns over the environmental impacts of plastic wastes have amplified the need for innovative strategies to achieve a circular plastic economy, ensuring a sustainable solution.^{1,2} Upcycling, which involves converting waste materials into higher-value products, presents a promising approach to reducing the environmental burden of plastic wastes.³ Building upon our ongoing research on developing zeolites, as documented in prior work⁴, this study focused on another zeolite-based catalyst for plastic wastes upcycling by keeping zeolite confinement intact while improving pore diffusion, overcoming key limitations in current cracking techniques. Through catalytic pyrolysis experiments on various polyethylene types, the superior performance of synthesized mesoporous zeolites, particularly for highly branched polymers, was demonstrated, emphasizing the role of pore architecture. Analytical techniques such as NH₃-TPD and *in-situ* DRIFT spectroscopy showed the critical function of Brønsted acid sites in boosting degradation efficiency. The optimized mesoporous zeolite catalyst, M720_{cit}, exhibited excellent efficiency in lowering degradation temperatures for a wide range of real plastic wastes. This research addressed key challenges in zeolite confinement and pore diffusion enhancement, contributing to the energy economic, and environmental sustainability of plastic wastes conversion processes.

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Hydroxide Ion Conduction through Viologen-based Covalent Organic Frameworks (vCOFs): an Approach towards the Advancement

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Abstract

Alkaline fuel cells rely on the movement of hydroxide anions (OH^-) for their operation, yet these anions face challenges in efficient conduction due to their limited diffusion coefficient and substantial mass compared to proton (H^+) transport. Within the covalent organic framework structure, ordered channels offer a promising solution for OH^- ion transport. Herein, we synthesized a cationic covalent organic framework (vTAPA) via the solvothermal-assisted Zincke reaction. vTAPA showcases excellent stability in harsh basic solution (12M) and a wide pH range. This framework facilitates OH^- conduction through its one-dimensional network through the anion exchange process. We employed various tertiary ammonium salts (tetramethyl-, tetraethyl-, and tetrabutyl- ammonium hydroxide) to exchange trapped anionic chloride ions inside the vTAPA structure with OH^- ions. The DFT study exhibited that the anion exchange process is very favorable as the vTAPA framework offers preferable interaction sites for OH^- ions. The impact of steric hindrance from these tertiary ammonium salts on OH^- conduction performance was extensively investigated. Butyl@vTAPA exhibited high OH^- ions conductivity of $1.05 \times 10^{-4} \text{ S cm}^{-1}$ at 90 °C under 98% relative humidity (RH). Our uniquely designed cationic COF created a platform for a preferential transport network of hydroxide ions and this is the first report of directly used COFs for hydroxide ion conduction without any vigorous post-synthetic modification.

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Disorder-Induced Hierarchical 4,4'-bipyridine based Macro/meso Porous Ionic Covalent Organic Framework for The Efficient Removal of Toxic Pollutants from Water

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Abstract

The rational design and synthesis of macroporous framework has immense importance in addressing basic obstacles in materials science and providing effective solutions for the removal of harmful pollutants from water. Here, a novel p-toluenesulfonic acid assisted the mechanochemical approach is used to prepare a 4,4'-bipyridine-containing ionic covalent organic framework (iCOF), which can be further converted into 3D foam architecture (named as L₃Tp@FOAM) by introducing a disorder through in situ gas-phase foaming technique using NaHCO₃ as a forming agent. The presence of high-density defects in the hierarchically porous structure along with exchangeable chloride counter anions in the L₃Tp@FOAM framework ensures the ultrafast capture (<10 sec) of various toxic pollutants from water, which can be benefitted for the mankind. L₃Tp@FOAM displayed an efficient removal (~99% removal) to a wide range of inorganic/organic species including MnO₄⁻, CrO₄²⁻, ReO₄⁻ and HAsO₄⁻, as well as organic dyes like Methyl Orange, Alizarin red, and Crystal Violet within very less timeframe. The oxoanions, such as MnO₄⁻, CrO₄²⁻, ReO₄⁻ and HAsO₄⁻, exhibited a high absorption capacity, even in the presence of other interfering anions. Among all four anions, MnO₄⁻ exhibited the maximum absorption of 920 mg g⁻¹ which is the highest among the reported reports to date. Further L₃Tp@FOAM effectively adsorbs anionic dyes such as Methyl orange, Congo Red, and Alizarin Red within a 30 sec timeframe, achieving a ~99% removal rate. This novel three-dimensional foam composed of ionic covalent organic compounds (L₃Tp@FOAM) has been investigated for the very first time, and it exhibits remarkable and exceptional efficacy in removing harmful pollutants from water, which can be comparable with reported materials.

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Triphenylamine based Covalent organic Framework foam for the Efficient Removal of Toxic Oxo-anions from Water

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Abstract

Covalent Organic Frameworks emerged as an alternative adsorbent material for oxoanion removal due to its high adsorption capacity, wide surface area, tunable porosity, porous structure, and recyclability. The present study involved the synthesis of a BPTP framework based on triphenyl amine. This was achieved using two different methods: a gas-forming technique employing ball mill approach (BPTP@FOAM), and a solution suspension approach at room temperature (BPTP@RT). Following that, this molecule was employed to examine the elimination of oxoanions, specifically the CrO_4^{2-} and MnO_4^- ions, from water. Due to the simple diffusion of oxoanions through the disordered 3D architecture of BPTP@FOAM, disorder-induced BPTP@FOAM was more efficient than the corresponding BPTP@RT. The BPTP@FOAM exhibited a remarkable 98.8% efficiency in eliminating CrO_4^{2-} ions during 30 min, and a notable 98% efficiency in removing MnO_4^- ions within a shorter duration of 10 minutes. This result is similar to several techniques that have been reported. The removal of CrO_4^{2-} ion and MnO_4^- ion in the presence of other competing ions and in wider pH range was conducted in order to verify their real-time application. A very advanced computational analysis was performed to investigate the interaction between the framework and Oxoanions.

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Development of Lignin based Bimetal oxide Nanocomposites for Waste Water Treatment

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Abstract

Water scarcity has become one of the pressing challenges across the globe. Removal of common microbes and organic pollutants is one of the sustainable ways to restore water. Valorizing biodegradable raw materials derived from agri-waste is ecologically beneficial. Employing such materials to produce nano-adsorbents and nano-photocatalyst is a smart platform for applications in wastewater treatment. Lignin is one of the most plentiful natural biopolymers in the world. Its macromolecular structure possesses phenolic and carboxyl groups that can capture heavy metals and dyes. Lignin can be chemically and physically modified to generate adsorbent and photocatalytic nanomaterials with enhanced capacity to remove pollutants from wastewater. A green synthetic approach was utilized to fabricate the nano-photocatalyst and nano-adsorbent with lignin as a tool to valorize agri-waste. Lignin has been used as a natural resource to synthesize lignin-metal oxide/bimetal oxide-based nano-adsorbents and nano-photocatalyst. The synthesized lignin based green nanomaterials effectively removed common pollutants from wastewater including dyes, heavy metals, and bacteria. The lignin-based water purification technique holds potential to effectively remove the most common pollutants from wastewater. The showcased methodology used especially agri-waste and has the enormous potential to be a dependable and sustainable strategy for drastically reducing the most prevalent large-scale water pollutants.

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Highly Crystalline n-p Heterojunction AgBr-NiO for the Organic Contaminant Degradation, Mineralization and Bacterial Eradication

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Abstract

A simple one-pot method was used to synthesize a novel AgBr-NiO compound and highly efficient photocatalysts. SEM and TEM analyses indicated that AgBr NPs with NiO form a spherical shape and are highly crystallized, as proven by XRD and SAED. While EDX and XPS analysis confirms the presence of corresponding elements (O, Ni, Ag, and Br) in the heterostructure, proving the high purity of the AgBr-NiO produced. The BET analysis reveals the mesoporous behavior of the AgBr-NiO heterostructures and performed better photocatalytic degradation under visible light for Rhodamine (RhB) & Bisphenol A (BPA) than the bare samples. The increase in fast light absorption and efficient photo-generated electron/hole pairs results to high photocatalytic activity for RhB (97.6% in 11 min) and BPA (85 % in 120 min). The kinetics study of photodegradation reveals that it follows first order reaction kinetics. Furthermore, the photo-mineralization of both compounds under investigation was studied by TOC depletion under analogous reaction conditions. Trapping experiments were performed to investigate the involvement of ROS during the degradation process. A feasible Z-scheme mechanism has been proposed to explain the production of the e^-/h^+ pairs under visible light and to promote spatial charge separation by tandem n-p heterojunction.

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Redefining Photocatalytic Systems with Heterobimetallic [Fe^{II}Ir] Complex: Role of Second Metal

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Abstract

The development of innovative, efficient photocatalysts is becoming an exciting trend in catalysis. Traditionally, most designs were centered on Ru(II) complexes, but their potential for exploration was limited due to the rapid relaxation of excited states into a non-emissive metal-centered (³MC) state.¹ Ir(III) complexes, however, emerged as far superior alternatives, providing greater ligand field stabilization energy and allowing for more effective manipulation of the lowest unoccupied molecular orbital by introducing different organic moieties.² Yet, the introduction of a second metal in these systems remains an untapped area of research. Ferrocene (fc), with its extraordinary structural and electronic properties, has proven to be a highly effective redox mediator. In this context, a heterobimetallic Ir(III) complex, [Ir(ppy)₂(fcbpy)]PF₆ (ppy = 2-phenylpyridine; fcbpy = 4-ferrocenyl-2,2'-bipyridine), was synthesized and its structure established by single crystal XRD.³ The high lifetime of 592 ns is the key feature where 390 ns lifetime of the similar iridium complex without fc. This complex demonstrated catalytic efficiency in visible-light-driven coupling reactions involving α-ketovinylazides and N, N-dimethylanilines. The iridium complex without fc failed to provide any desired product. Additionally, a Fe^{II}/Ir-dye-loaded Pt/TiO₂ system was carefully designed and synthesized for applications in solar hydrogen production. A process that generates clean, renewable energy (H₂)⁴ without producing environmental pollutants, highlights the importance of sustainable and eco-friendly solutions in energy generation.

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Removal of Toxic Oxo-Anion Pollutants from Water by Using Cationic Imide Covalent Organic Framework

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Abstract

Over the past years, there has been a flurry of activity in the field of water detoxification using ionic porous materials. These materials have a lot of appealing properties, like being easy to synthesize, scalable, and effective in removing contaminants from wastewater. This work is all about the synthesis of cationic imide covalent organic framework using Triaminoguanidinium chloride (TGcl) and Naphthalenetetracarboxylic dianhydride (NTDA). This results NTDA-GAC imide COF with high stability and eye-catching porosity. This COF is the first ionic COF in Imide COF area. By using this COF, we have achieved a good range of adsorption of pollutants (MnO_4^- , CrO_4^{2-} , HAsO_4^-) from drinking water. MnO_4^- showing the highest capture capacity among all the pollutants.

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Selective Capture of Bromine over Iodine by a Nanometer-Sized Covalent Organic Framework Containing Imines and Hydrazones

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Abstract

The storage and transport of elemental bromine is challenging due to its volatile, toxic and corrosive nature, making efficient bromine removal a critical area of research.^{1, 2} Traditional Br₂ capture materials often suffer from problems such as instability in water and poor halogen retention.^{3, 4} In response, we present a facile, scalable synthesis of a nanoscale covalent organic framework (COF-2H1) that effectively removes bromine from a variety of media. This high efficiency is due to favourable interactions between bromine and the π -electron-rich imine and hydrazone bonds within the COF-2H1 structure. The material exhibits high bromine uptake capacities of 11.29 g/g from water and 15.34 g/g from cyclohexane, outperforming previous bromine adsorbents. In addition, COF-2H1 can selectively capture bromine over iodine from halogen mixtures, addressing a significant challenge in industrial bromine remediation, particularly from mixtures of bromine, iodine and interhalogen compounds such as IBr. This selective capture makes COF-2H1 a promising solution for obtaining pure bromine, offering a stable and efficient approach to bromine removal and remediation processes in industrial applications.

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High-Performance Cobalt-Phosphonate Nanoparticles for Cycloaddition Reactions: Synthesis, Characterization, and Industrial Catalysis of Cyclic Carbonates

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Abstract

Herein, we report the synthesis of Cobalt-phosphonate nanoparticles through the simple chemical reaction between two phosphonate sources (PPA & EDTMPS)¹⁻³ and Cobalt nitrate hexahydrate under hydrothermal conditions. Here the materials were characterized using FT-IR, P-XRD (powder X-ray diffraction), FE-SEM, TGA, XPS, HR-TEM, and, Brunauer–Emmett–Teller (BET) surface area measurement. In this study, we focused on the effects of the organic functional groups for effective catalytic ability. Interestingly, Co-EDTMPS demonstrates crystallites of smaller size and higher surface area than Co-PPA. Due to the presence of basic group nitrogen in Co-EDTMPS. The Co-EDTMPS catalyst exhibited higher catalytic performance with conversion = 99%, selectivity = 99%, and yield = 99% without using any solvent at optimized conditions such as catalyst = 10mg, Co-catalyst (TBAB) = 10mg, pressure 7bar, temperature = 100°C, Time = 24h.⁴ These materials showed high catalytic activity for the synthesis of cyclic carbonates from a wide range of different epoxides in the presence of CO₂ at atmospheric pressure. NMR and GC-MS techniques were used to reveal the plausible mechanisms and revealed the direct preparation of cyclic carbonates without any by-product formation. The characterization of the used catalyst, easy recoverability, and the ability to be recycled over five times with more than 90% conversion demonstrate its ability to be used as a suitable catalyst for industrial purposes.

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Pickering Interfacial Catalysis – A Novel Concept for Green Synthesis

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Abstract

Pickering emulsions are the dispersion system of two immiscible liquids stabilized by solid particles. If the Pickering solid also acts as a catalyst in a chosen reaction, the process is known as Pickering interfacial catalysis (PIC). The advantage of PIC is that reactants that are not water soluble and hence require an organic solvent can be made to occur in an emulsion system containing water. Since the stabilising solid itself acts as a catalyst, the process also reduces the use of multiple reagents. In this study, MgO prepared through various methods and characterized using XRD, FESEM, HRTEM, DLS, and CO₂-TPD techniques, was used as an emulsion stabilizer and also a catalyst for Knoevenagel condensation. The effect of particle shape on the PIC was investigated. Results indicate that the emulsions stabilized by rod and plate-shaped MgO particles exhibit higher stability and catalytic activity compared to other MgO samples. Furthermore, the MgO-PIC system also demonstrated successful gram-scale synthesis (85 % yield in 30 min). The catalytic system is also reusable for at least five cycles with minimal loss in activity.

Effect of Lignocellulosic Component Precursor on the Property of Activated Carbon through Chemical Activation

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Abstract

In this study, lignin, as component of lignocellulosic biomass, was investigated as a precursor for activated carbon production. The experimental focus was on mixing lignin with potassium hydroxide (KOH) in certain ratio under pyrolysis conditions. The process was carried out at distinct temperatures with a fixed residence time and a heating rate. The KOH-treated lignin, pure lignin was also subjected to pyrolysis at the same temperatures to compare the property of prepared carbon material. This research aimed to examine how the temperature and the presence of KOH influence the physical and chemical properties of the resulting carbon material, such as its structural morphology, surface area, and porosity^[1]. The analysis highlights the effects of temperature variation on the yield and quality of carbon, offering insights into the optimization of lignin for applications in energy storage system and environmental remediation^[2]. By utilizing lignin, a by-product of biomass, in the production of valuable carbon materials, this study contributes to advancing sustainable material science, aligning with the growing demand for renewable and eco-friendly alternatives in industrial processes.

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Incorporation of Palladium Telluride Nanoparticles over Amine Functionalized NH₂-UiO-66 Metal-Organic Framework (MOFs): Synthesis, Characterization and Application in Water Splitting Reaction

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Abstract

Many persistent and low-cost pesticides are regularly used for domestic, agricultural, and industrial purpose. Bioaccumulation and toxicity of pesticides have raised environmental concerns, highlighting the need for effective removal techniques by using nanomaterials. The ability of hybrid nanocomposites of ZnO@CdS were utilized for the removal of hazardous and chlorpyrifos (CP) and atrazine (Atz) pesticides. A green methodology using *A. indica* (commonly found plant in India) leaves extract employed as a natural surfactant and deionised water as a solvent for the synthesis of ZnO@CdS nanocomposite. The purity and crystallinity of the deformed spherical nanoparticle (10–80 nm) were ensured by the sharp peaks acquired by PXRD. Subsequently, ZnO@CdS nanocomposite was investigated for the elimination of pesticides at discrete reaction parameters (catalyst: 10–35 mg; pollutant: 2–10 mg/L for CP; 50–250 mg/L for Atz mgL⁻¹; pH: 3–11, dark-sunlight). ZnO@CdS nanocomposite showed maximum degradation with 50 mg catalyst dose, 2 mgL⁻¹ of at neutral pH in the presence of daylight. Results of BET (111 m²g⁻¹), zeta potential (-40.5 mV), and bandgap (1.67 eV) also supported the effective photocatalytic efficiency of ZnO@CdS nanocomposite. Safer metabolites formed after degradation confirmed by GC-MS analysis. Finally, the ZnO@CdS nanocomposite may be a viable alternative catalyst for industrial applications due to its high surface activity, stability, charge separation, and reusability (n = 8).

Cu-Catalyzed Sustainable Synthesis of [1,2,3]triazolo[1,5-c]quinazolin-5(6*H*)-one Heterocycle Derivatives via Sequential Reaction of Ethyl-2-(2-oxoindolin-3-ylidene)acetate with Sodium Azide

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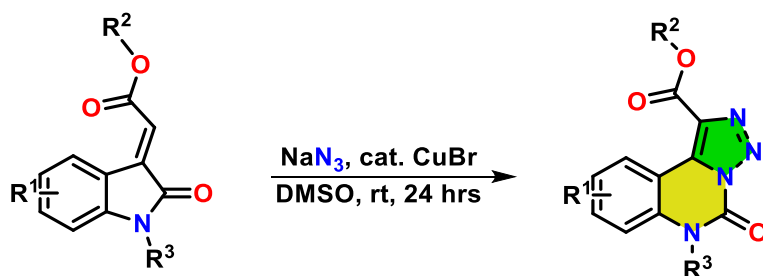
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Abstract

N-Heterocycles are immense interest in medicinal chemistry and also widely used scaffold in the pharmaceutical applications. Diverse heterocyclic structures were also found in many naturally existing alkaloids that are used as drugs for various applications. As a result of wide-range of applications,^{1,2} several synthetic approaches to create a variety of complex heterocyclic molecules were demonstrated in the past several decades. Further, new approaches with modern demands have been fascinated by synthetic organic chemist over the years. N-fused heterocyclic compounds with quinazoline and triazole frameworks, including triazolo[1,5-c]quinazoline have drawn much interest from both medicinal and synthetic chemists.

Herein, we have successfully developed a novel, simple and efficient method for the synthesis of 5-oxo-5,6-dihydro-[1,2,3]triazolo[1,5-c]quinazoline. The method is based on the copper-promoted reaction of α , β -unsaturated keto/ester methyleneindolinone with sodium azide in room temperature through an azide-alkene cyclization and rearrangement ring expansion which is applicable to a variety of α , β -unsaturated keto/ester methyleneindolinone. The reaction displayed wide functional group tolerance and demonstrated in gram scale applications and the process have high atom-economy. A detailed mechanism has been postulated with the experimental evidences.



- Mild Reaction Conditions
- Broad substrate Scope
- Regio-selective ring expansion

- Good to excellent yield
- New heterocyclic Framework
- Could be a potential anti-malarial agent

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Mesomorphic and Dielectric Properties of Strategically Designed Chiral Bent-Core Liquid Crystals Displaying Wide Temperature Range Dark Conglomerate Phase

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Abstract

In order to advance the scope of chiral functional materials, it is of paramount importance to engineer chiral bent-core liquid crystals (LCs) endowed with exceptional stability across a broad range of temperatures. In this context, we have devised a strategic approach, utilizing the potential of fluorinated molecules and taking advantage of the chirality of cholesterol as the pivotal component. This synergy has enabled the successful synthesis of our target LCs **nF-4R**. These molecules exhibit a chiral dark conglomerate (DC) phase over a broad temperature range of B85 1C in an enantiotropic manner. Dielectric spectroscopy measurements conducted on these materials showed persistent dielectric behavior over the entire LC range. Our study stands as a pioneering exemplar, unveiling the wide-range DC phase within the intricate landscape of chiral bent-shaped molecular systems. The mesomorphic characterization utilizing polarized optical microscopy, differential scanning calorimetry, and smallangle/wide-angle X-ray scattering measurements, revealed an optically isotropic DC phase. This phase shows domains of opposing chirality and belongs to the sponge-type DC phase. Notably, the enhancement of a specific chiral domain reveals the bias towards supramolecular chirality, attributable to molecular chirality as supported by circular dichroism measurements. This finding holds promise for chiral plasmonics, enantiomeric separation, and nano-templating applications.

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Open Loop Upcycling of Polyethylene Terephthalate Waste to Valuable Chemicals Catalyzed by Co₂P Anchored on TiO₂

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Abstract

Ever increasing usage of plastic commodities due to their low cost, easier availability, high durability, etc., has led to a tremendous increase in the generation of plastic waste. Among the primary plastic pollutants, polyethylene terephthalate (PET) holds major shares in the packaging industry and is responsible for global plastic waste production per annum. Therefore, chemical upcycling of PET plastic waste into valuable chemicals is a field of utmost importance aiming at a circular economy. In this work, we have developed a composite of cobalt phosphide anchored on titania oxide for efficient synthesis of morpholine amide from direct PET flakes (88% yield) as well as terephthalic acid (90% yield). The TPA was obtained from the neutral hydrolysis of PET with 94% yield under environmentally benign conditions with detailed optimizations of the methodology. Morpholine Amide holds a potential utility as a building block in organic synthesis which has been examined by further deoxygenation reduction reaction to form benzylic amine (77% yield). The synthesized Co₂P-TiO₂ catalyst exhibits excellent stability and catalytic activity in the aminolysis of PET flakes for multiple reaction cycles. Moreover, the green metric parameters were calculated for both neutral hydrolysis and aminolysis reactions to analyze the sustainability of the developed reaction protocol. Therefore, such effective and efficient strategies integrating depolymerization and upcycling of real-world PET plastic waste can serve as a highly advantageous approach for large-scale industrial realization.

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Green Approach for the Synthesis of Acrylonitrile Hyperbranched Polymer/Chitosan for the Uptake of Diclofenac from Water by using Box–Behnken Design (BBD) under Response Surface Methodology (RSM).

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Abstract

Acrylonitrile hyperbranched polymer/chitosan composite (AC-Hyp/CS) material was synthesized for the removal of diclofenac. In this method a hyperbranched polymer was prepared by the crosslinking of acrylonitrile monomer to get a host with a wide surface area (AC/Hyp). To improve the functional sites of the AC/Hyp is functionalized with chitosan (AC-Hyp/CS) which leads to the excellent removal efficiency. The physiochemical characterization of AC-Hyp/CS was carried out by FTIR, XPS, PXRD, DLS and SEM coupled with EDS. The uptake of diclofenac onto AC-Hyp/CS was optimized by RSM in combination of BBD. The isothermal and kinetic models were applied which suggested that the Langmuir isotherm model was administrated well with equilibrated data as it shows appropriate R^2 values (0.9814–0.9908) and low values of error functions (SSE: 0.002–11.742, χ^2 : 1×10^{-5} –0.048). The adsorption capacity (maximum) obtained from Langmuir model was found 200 mg g⁻¹ and pseudo-second-order kinetic model confirmed that the absorption was chemisorption because of high values of R^2 (0.9878–0.9982) and low values of error functions (SSE: 0.160–1.343, χ^2 : 0.004–0.053). The investigation of adsorption/desorption cycling test suggested that had excellent reusability characteristics upto 7 cycles which agreed that the AC-Hyp/CS could be an effective sorbent for elimination of diclofenac from aqueous environment.

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Surface Functionalized Hollow Fiber Membrane for Separation of Liquid mixtures

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Abstract

Membranes selectively separate or limit the transport of specific phases. Their development for applications like separation, adsorption, desalination, and filtration is a key area in chemical engineering and materials science. Researchers are investigating polymer, glass, ceramic, and composite membranes for their scalability¹. However, polymers often struggle under high temperatures and harsh conditions. Ceramic hollow fiber membranes, with superior resistance to abrasion, chemicals, and heat, are ideal for such environments. Surface-modified ceramic membranes can be used for environmental applications like wastewater treatment, desalination, metal separation from waste batteries and gas purification. So we develop ceramic hollow fiber membranes for separation by surface functionalisation. We are modifying these fibers for oil water separation². Moreover, zeolite coated hollow fiber for azeotropic mixture separation.³

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Sequential Cycloisomerization and Diels's -Alder Reactions to Access Octahydroquinoline Scaffolds

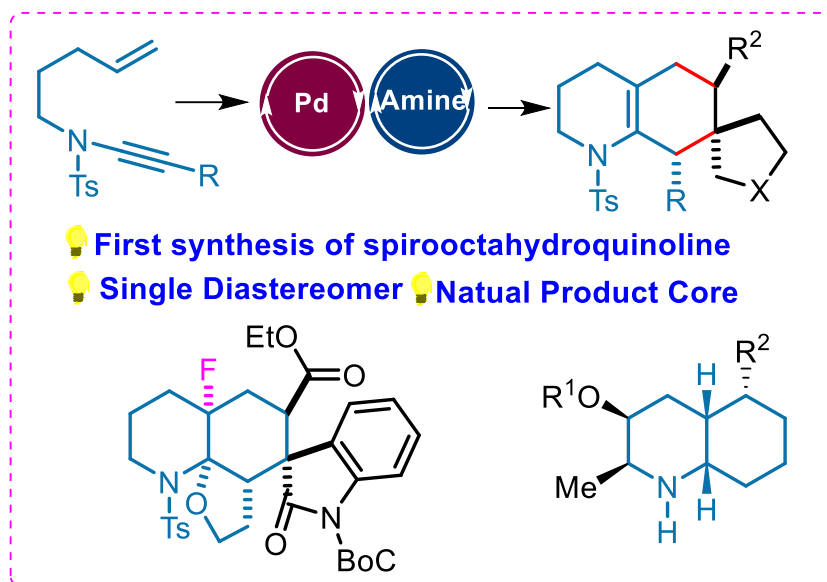
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Abstract

This presentation addresses the synthesis of octahydroquinoline frameworks through a Pd-catalyzed enynamine cycloisomerization¹⁻² and by an amine-catalyzed Diel's-Alder reaction³⁻⁴ sequence, in a highly stereoselective fashion. The method culminates the synthesis of >35 examples of the targeted adducts, achieving high yields and exceptional diastereoselectivity (>99:1 dr). Furthermore, the practical applicability of this approach is demonstrated *via* a two-pot, three-step procedure resulting in spiro-, tricyclic decahydroquinoline⁵ architecture that closely resembles Lepadin alkaloids.



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Synthesis and Characterization of Zn and Cu Dopped MnFe₂O₄ Multinutrient Nanofertilizer And it's Field Application on Growth Performance of Chilli (*Capsicum Annuum L.*)

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Abstract

Recent research has focused on the synthesis and characterization of MnFe₂O₄ nanocrystals doped with zinc and copper. This synthesized material serves as a multinutrient nanofertilizer in agriculture, promoting improved crop growth and seed germination. The doping of Zn and Cu into MnFe₂O₄ was achieved using the sol gel technique, with annealing conducted at 800°C for four hours. Characterization was performed by using XRD and SEM-EDAX to analyse the structure, crystallinity and morphology of nanoparticles. The XRD results revealed peaks corresponding to Zn and Cu into MnFe₂O₄, confirming spinal cubic phase, as noted in ICDD card number 75-0034. The Zn and Cu dopped MnFe₂O₄ was applied as a multinutrient nanofertilizer to enhance growth performance of chilli. Results indicated that the Zn and Cu doped MnFe₂O₄ significantly improved the seed germination, chlorophyll content, and morphological characteristics of the chilli crop by supplying essential micronutrients like zinc, copper, manganese and iron to agricultural crop.

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Theoretical Investigation on Photoinduced Host Guest Electron Transfer and Ultrafast C–H Bond Activation

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Abstract

C–H activation without the use of metal-based catalysts is crucial because it offers a more sustainable and environmentally friendly approach to chemical synthesis. In this study, using a detailed theoretical /computational investigation we shed light on the underlying mechanistic facets of the recently reported case of visible light-mediated charge separation-based oxidation of toluene and its congeners through C–H bond functionalization within organic and metallo-organic nanocavities. Our findings highlight the significant role of photoinduced host guest electron transfer in weakening the traditionally inert C–H bond, which is characterized by low bond polarity and high dissociation energy. Through ab initio/TDDFT and DFT calculations on toluene within the nanocavity, we elucidate how excited state proton transfer and electron transfer processes facilitate the selective oxidation of the C–H bond, resulting in benzaldehyde formation as the predominant product in the presence of oxygen.

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NiAl-Layered Double Hydroxide Catalyst for Catalytic Transfer Hydrogenation of Benzaldehyde

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Abstract

Development of green and sustainable protocols for carrying out transfer hydrogenation reactions has been a challenging task due to low activity of non-noble metal-based catalysts. Layered double hydroxides have turned out as promising catalysts for the catalytic transfer hydrogenation due to the presence of large number of basic sites, scalable, and fast synthesis. In our work, a highly efficient NiAl LDH catalyst was synthesized by the conventional co-precipitation method. The as-synthesized catalyst turned out to be highly efficient for the catalytic transfer hydrogenation of benzaldehyde to benzyl alcohol. Further, optimizations were carried out by varying different parameters (catalyst amount, temperature, time and hydrogen source). The developed protocol was further extended to transfer hydrogenation of different substrates to investigate the role of different substituents. The structure activity relationship was also examined which suggested that the basic sites play major role in the catalytic transfer hydrogenation. Also, green metric parameters were calculated in order to investigate the greenness of the developed protocol. This study proved that the developed protocol turns out to be green, sustainable and highly compatible for carrying out the transfer hydrogenation in relatively mild conditions.

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Enhancing Soil Quality through Nanoparticle Amendments

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Abstract

As a CO₂ mitigation approach, soil organic carbon (SOC) storage in terrestrial ecosystems, particularly wetlands, has gained attention lately. SOC is a crucial factor that affects soil C balance and dictates the productivity and quality of the soil.^[1] But, in recent years anthropogenic activities have led to a depletion in SOC in ecosystems on a global scale. In this sense, soil carbon must be recovered whenever possible to minimize the environmental impact, using sustainable remediation strategies. Nanotechnology is widely used to address environmental challenges, especially when it comes to employing nanoparticles (NPs) for site cleanup. At first, these nanomaterials were only used to clean up water contaminated by metal(loid) pollutants.^[2] This study examined the effects of metal NPs and their dissolved ions on the microbial community composition, enzyme activity and organic carbon levels in a wetland soil. The outcome shows how NPs can impact soil enzyme activity, microbial community composition and soil carbon upon introduction into soil, depending on their type, concentration, and dissolution behaviour, hence providing much needed information for the sustainable application of nanotechnology in this field.

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Fine-Tuning B-Ketoenamine based Covalent Organic Frameworks for Structure-Activity Correlation for Iodine Adsorption Studies

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Abstract

Radioiodine isotopes (^{129}I and ^{131}I), as nuclear waste, pose serious health and environmental risks. ^{131}I can cause acute health issues like thyroid cancer due to its rapid absorption by the thyroid, while ^{129}I remains in the environment for millions of years, contaminating water and biodiversity. Given these dangers, Covalent Organic Frameworks (COFs) are a promising solution for iodine adsorption. Their high surface area, tunable pores, and functional groups enable efficient and selective capture of radioiodine. In this work we have introduced three isorecticular COFs—COP-N18 (covalent organic polymer with short-range order), COF-N18 (COF-N18 having long-range order), and COF-N27 (semicrystalline COF with pyridyl heteroatoms)—to explore the systematic variations in structural order, pore volume, and pore-wall nitrogen content. This study aims to establish a structure-property relationship for these COFs *via* iodine adsorption. Our investigation highlights the positive influence of crystallinity, surface area, and pore volume in iodine adsorption. COF-N18, with highest surface area (1262 m²/g) and pore volume (1.98 cc/g), demonstrated rapid iodine adsorption but had a lower overall uptake capacity. In contrast, COF-N27, despite its modest surface area (840 m²/g), exhibited a higher iodine uptake capacity (7.84 g/g). However, heteroatomic nitrogen-doping retards the adsorption rate through chemisorptive charge-transfer interactions. Finally, COP-N18 showed the least iodine uptake capacity, as it has the lowest surface area and pore volume. Our study underscores the balance between crystallinity, porosity, and the role of active sites in iodine adsorption, offering valuable insights for the strategic design of COFs in nuclear waste management.

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Multi-Stimuli Responsive Functionalized Boranil Fluorophores and their Potential Application as a Re-Writable Material

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Abstract

While many conventional boron complexes suffer from aggregation-caused quenching, a rational molecular design is essential for creating solid-state emissive fluorophores from a basic core structure. We have developed a series of solid-state emissive boranil-based complexes and investigated their spectroscopic properties in the solution and solid state. The structural features of the synthesized complexes are responsible for their mechanochromic properties. Upon mechanical grinding, **B-PTPA** and **B-PPY** dyes exhibit emission shifts of 21 nm and 17 nm, respectively. Throughout the four cycles, both dyes showed outstanding reversibility after fuming/solvation with DCM in response to mechanical stimulation. Powder X-ray diffraction (XRD) revealed that the changes in solid-state fluorescence were due to the rearrangement of the crystal packing. The changes in the crystallinity were confirmed by DSC and Powder-XRD. These materials have been used as pressure sensor, information storage,¹ optical displays,² chemical sensors,³ and security ink⁴ related applications.

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A Pd (II)-Catalysed Denitrative Alkyne Annulation Reaction for the Synthesis of Cyclopenta[b] Chromanes

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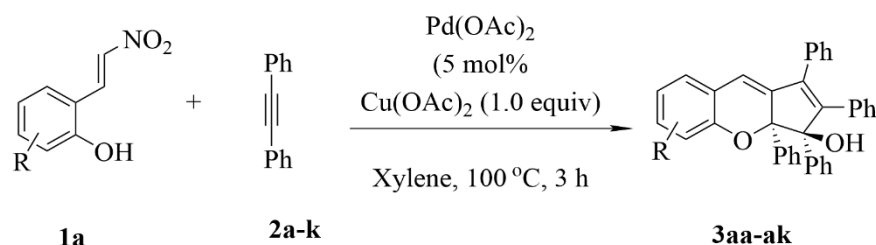
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Abstract

An unprecedented Pd(II)-catalyzed annulation reaction is developed for the synthesis of cyclopenta(b)chromane derivatives bearing a tertiary hydroxyl group. In this reaction, readily available 2-(2-nitrovinyl) phenols are annulated with two molecules of disubstituted alkynes via denitration to afford a wide range of annulated products. Additionally, one novel In(III)-catalyzed dehydroxylative 1,2-phenyl shift reaction is also performed on some of the synthesized chromane derivatives to afford cyclopentenones



Polydispersity Mastery: Zeolite Crystal Control via Cation-Mediated Colloidal Silica Stabilization

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Abstract

Tailoring the physical properties of advanced functional materials is vital for enhancing their performance across various applications. This requires a deep understanding of their formation mechanisms. In this study, we focus on the industrially significant zeolite, SSZ-13, widely used in processes like Selective Catalytic Reduction and the Methanol to Olefin reaction. Controlling the polydispersity, size, and morphology of zeolite crystals has been challenging for catalyst design. To address this, we developed a novel synthetic method for SSZ-13 crystals, allowing precise control over particle size, dispersity, and morphology. This method utilizes cost-effective modifiers, making it commercially viable. By altering the physicochemical conditions of the mother liquor, we synthesized crystals with varying sizes and improved dispersity. We examined the impact of different salts (monovalent, divalent, trivalent) as counter ions or stabilizers on crystal growth. The addition of cations influenced particle size and growth dynamics by forming a hydrosphere that hindered the diffusion of aluminate and silicate species, suppressing growth. Without modifiers, crystals displayed a bimodal distribution. Using monovalent cations produced ~500 nm crystals, while bivalent cations resulted in ~2 μm monodisperse populations. Trivalent cations led to morphological changes. Our study provides a detailed mechanism and a complete library of controlled particles.

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Influence of Different Surfactant Combinations and Antioxidant Mode of Incorporation on the Oxidative Stability of Castor Oil-In-Water Emulsions

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Abstract

Now-a-days, there is a very high demand to inhibit lipid oxidation at interfacial region of emulsions by modulating the mole fraction of surfactant mixtures and selecting appropriate and effective antioxidant. In this context, we hypothesized to bring novelty in our work by using a mixture of differently charged nonionic and zwitterionic surfactants in intact castor oil-in-water emulsions for the first time to modify their interfacial region for the determination of the oxidative stability of its unsaturated fatty acids. Here, we carried out the interfacial kinetics studies by employing the pseudophase kinetic model to evaluate the distribution of antioxidant, tertiary butylhydroquinone (TBHQ) between the different regions of emulsions and the second order interfacial rate constant (k_I) for the reaction between 4-hexadecylbenzenediazonium ion (16-ArN_2^+) and TBHQ. Studies carried out on emulsions prepared from different mole fractions of Tween 20 and 3-(N,N-Dimethylmyristylammonio)propanesulfonate (DPS) display that there is a direct correlation between the different mole fractions of surfactants and the distribution of antioxidant between different the regions of emulsions along with an interesting outcome that DPS brings more TBHQ towards the interface as consequence of tunable acidity, which in turn quenches the lipid oxidation at the interface to a considerable extent. Thus, our observations are promising in making remarkable impacts on the food and pharmaceutical industries as one gets the knowhow of efficient antioxidants to be used for enhancing the shelf life of particular food system.

Synthesis, Structural Analysis, and Antibacterial Properties of New Fluorinated Pyrazoline Derivatives

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Abstract

The pharmaceutical and organic industries have advanced the use of pyrazolines, nitrogen-containing five-membered heterocyclic compounds, also referred to as pyrazoles. This study focuses on synthesizing and characterizing a new series of 3-(4-fluoro-3-methylphenyl)-5-phenyl-4,5-dihydro-1H-pyrazole (FMPDHP) derivatives. Two synthetic routes were explored: one from chalcones and the other from hydrazine hydrate. In the first method, chalcones were prepared using 4-fluoro-3-methylacetophenone and substituted chlorobenzaldehydes through Claisen-Schmidt condensation at room temperature. In the second step, nine FMPDHP derivatives were synthesized from different substituted chalcones using hydrazine hydrate, glacial acetic acid, and anhydrous ethanol via an intramolecular Michael addition. The structures of these new compounds were confirmed using ¹H NMR, FT-IR, and HR-MS spectroscopy. The antimicrobial activity of derivatives 2a-i was tested against various pathogens, including *Escherichia coli*, *Staphylococcus aureus*, *Bacillus subtilis*, *Pseudomonas aeruginosa*, *Saccharomyces cerevisiae*, and *Candida albicans* by measuring the inhibition zones on discs treated with their DMF solutions. While compound 2c showed moderate activity, compounds 2h and 2b exhibited strong antibacterial properties. The influence of substituents on antibacterial effectiveness was also explored.

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Self-healing, Tough, Stretchable Ionogel for Energy harvesting

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Abstract

Ionogels have emerged as promising stretchable conductive materials, attracting significant interest in the field of flexible electronics[1]. However, developing ionogel-based devices that combine multiple desirable properties remains a crucial challenge[2-3]. The ideal ionogel-based device would integrate mechanical robustness, room temperature self-healing capabilities and ease of processing[4]. In this work, a self-healing, tough, stretchable ionogel is synthesized using a facile one-step process by the photopolymerization of acrylamide and acrylic acid in tributyl(methyl)phosphonium methylsulfate as solvent. The ionic liquid forms abundant and strong non covalent crosslink such as ion-ion and ion-dipole interactions and hydrogen bonding with polymer chains endows the ionogel enhances the mechanical properties along with fast self-healing ability at room temperature. Further, the prepared ionogel is used as a triboelectric layer for mechanical energy harvesting via triboelectric nanogenerator device.

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Synthesis of Carbon Quantum Dots (CQDs) from Biomass and Catalytic Application for Organic Synthesis

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Abstract

Carbon Quantum Dots have emerged as one of the most versatile and ignited domains, balancing the fundamental as well as applied research on a single podium. We hereby have synthesised CQDs from biomass waste *i.e.* banana peels and human hairs (B-CQDs and H-CQDs respectively) using Hydrothermal-(Bottom-Up approach), with the deep imprint of sustainable development and waste utilization.

Both these B-CQDs and H-CQDs have been comparatively scrutinized in order to set up a relation between the CQDs properties and the choice of precursor for their synthesis according to their application requirements. Characterizations including UV-Vis, ATR-IR, P-XRD, HR-TEM, EDX, SAED, etc. were performed to decipher the individual properties and behaviours from the gamut specialties of CQDs. The direct amino-acid functionalization of CQDs was unsuccessful but the intervening reason was disambiguated about the macromolecular synthon-tecton cluster cavity formation, which encapsulated CQDs and quenched their fluorescence properties. Diamine based functionalization of CQDs has also been investigated and the direct catalytic applicability of the H-CQDs and *f*-B-CQDs in organic synthesis of α,β -unsaturated compounds has also been explored and analysed via TLC and ¹H-NMR.

Room Temperature Synthesis of Nanoparticle @ Zr-MOF Core-shell Nanohybrid Facilitated by an Intermediate Polymer Coating

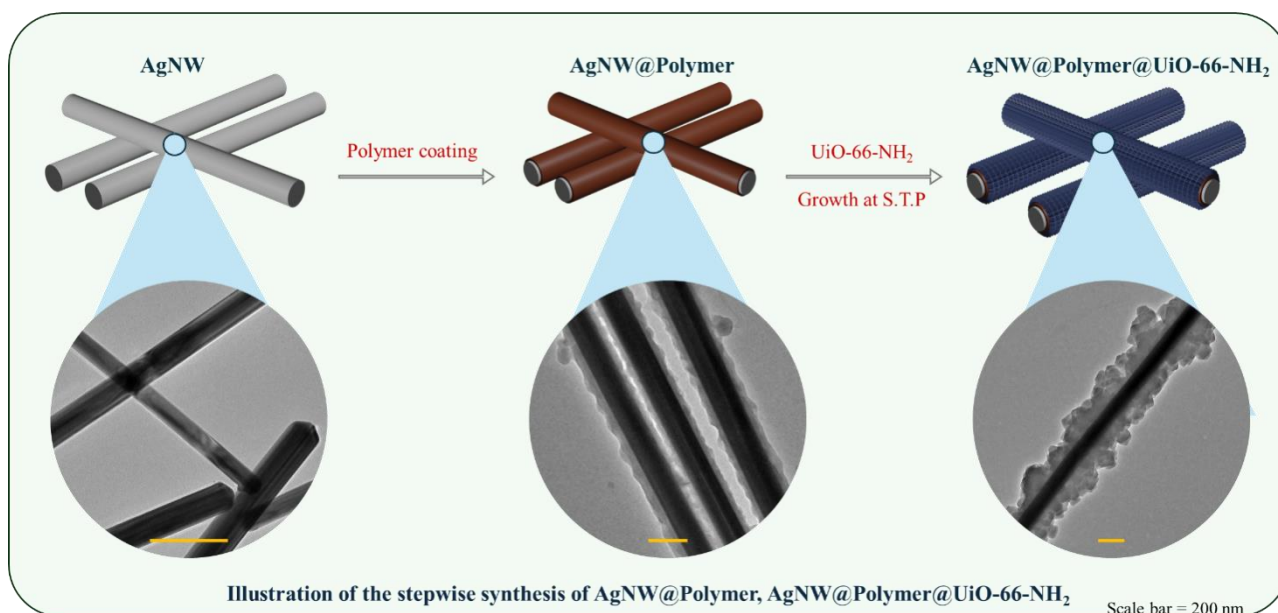
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Abstract

Core-shell nanohybrids with nanoparticles encapsulated in zirconium (Zr)-based MOFs are challenging to synthesize due to nanoparticle aggregation, often caused by high temperatures and salt-induced charge screening¹⁻². Here, we present an optimized room-temperature synthesis of a well-defined core-shell structure ($\text{AgNW@polymer@UiO-66-NH}_2$) with single nanoparticles as cores. We investigated the effects of key reaction parameters, including the flow rate of organic linker addition, linker concentration, and different polymer coatings. The increment in the flow rate of organic linker addition and its concentration at a fixed flow rate led to more free MOF formation along with the core-shell nanohybrid, attributed to rapid MOF nucleation from the rising bulk linker concentration, exceeding the optimum linker concentration for the formation of core-shell nanohybrid. Further, polymer coatings with functional groups such as amine, catechol (PDA), hydroxyl, carboxyl (CMC), and amide (PAM) promoted the chelation of metal ions and reduced interfacial energy, facilitating heterogeneous nucleation of MOF around the nanoparticles. The versatility of the developed synthesis method was demonstrated by employing 3D and 2D-shaped cores, achieving uniform core-shell nanohybrid in each case. This approach enables the development of nanohybrids for applications in sensing and catalysis, harnessing the synergistic properties of functional nanoparticles and MOFs



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Mechanistic Understanding of Morphological Evolution of Zeolite Synthesized via Solid-State Transformation

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Abstract

Zeolite has emerged as a prominent candidate in the multi-dimensional application field^{1,2} for its unique pore architecture and tunable acid site distribution. Conventional hydrothermal zeolite synthesis includes disadvantages like high amount of wastewater, low yield, high operational pressure, etc. To mitigate these challenges, researchers have recently developed a new pathway called solid-state transformation, a greener approach to synthesizing zeolite with high commercial profitability³. Although studies have successfully postulated the formation mechanism of several zeolite frameworks^{4,5}, the control over morphological growth and, hence, the intrinsic properties are still elusive. From this viewpoint, we have established a mechanistic insight into the process. A pure cancrinite framework was synthesized, and morphological evolution was tracked. Our investigation reveals the presence of a concurrent process where phase and morphological growth takes place simultaneously. Initially formed nanoparticles act as building units to undergo an agglomeration process to form a multipod-shaped bulk particle. Nanoparticles attach through a unidirectionally oriented crystallographic registry to form nano-domains. Different nanodomains have different common crystal planes. These nanodomains agglomerate randomly to form the final mesocrystal. A non-classical growth pathway was observed. Synthesized material with suitable morphology is chosen to perform CO₂ adsorption, breakthrough study, selective separation of H₂, and cyclic stability study.

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Fluorspar Activation in Water and the Synthesis of Fluorochemicals

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Abstract

Fluorspar (CaF_2) is the primary industrial source of fluorine, essential for producing pharmaceuticals, agrochemicals, and lithium-ion batteries.¹⁻³ Traditionally, extracting fluorine from CaF_2 requires treatment with sulfuric acid (H_2SO_4) at $\sim 300^\circ\text{C}$, generating highly hazardous hydrofluoric acid (HF).² Due to HF's extreme toxicity and corrosiveness, this process poses significant safety challenges and operational risks, with numerous accidents having occurred as a result. In this work, we introduce a novel method that bypasses HF generation while providing access to crucial fluorochemical reagents.⁵ Our approach employs a dual activation strategy: oxalic acid sequesters Ca^{2+} ions, while fluorophilic Lewis acids like boric acid ($\text{B}(\text{OH})_3$) or silica (SiO_2) capture fluorine by forming strong B–F (613 kJ/mol) or Si–F (565 kJ/mol) bonds. This method enables the synthesis of key fluorinated reagents, including tetrafluoroboric acid, alkali metal fluorides, tetraalkylammonium fluorides, and fluoro(hetero)arenes. This innovative process is scalable, operable under mild conditions, and can be safely executed in a standard laboratory without specialized equipment. Its potential to transform fluorine chemistry lies in its safer, more sustainable approach, which reduces the reliance on hazardous reagents.

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Development of Sustainable Multifunctional Silk Fabric using Exhaust Process

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Abstract

Releasing of wastes such as dredging, debris wastewater from various industries is the main supplement for the of source of growth of mosquitoes, germs, viruses, fungi, and free radicals which severely affect the health of human being. Commercially accessible synthetic pesticides (e.g., picaridin, permethrin, N, N-Diethyl-meta-Toluamide, etc.) help to control the growth of these insects and microorganism up to some extent. In comparison to synthetic pesticides, biomass-based sustainable material shows significant therapeutic qualities and eco-friendly nature towards to the environment. Additionally, a major part of the human body covered by fabrics, therefore attention has been paid to develop multifunctional fabrics for protecting humans from microbes, mosquito bites, and UV radiation. The exhaust process was used to

develop a multifunctional silk fabric by incorporating bioderived molecule (obtained from biomass), and biocompatible polyethylene imine. Fourier-transform infrared spectroscopy (FTIR) and field emission scanning electron microscopy (FESEM) analyses were used to reveal the functionality (chemical composition) and the morphology, respectively of as prepared fabric.

The result of mosquito repellent was achieved over 95% against *Aedes* species, and the antibacterial activity was found more than 99% against *S. aureus* and *E. coli*, and outstanding antioxidant activity and UV resistance (with a UPF rating >50)

Value Addition of Natural Products from Aromatic Crops: A Sustainable Approach for Drug Discovery

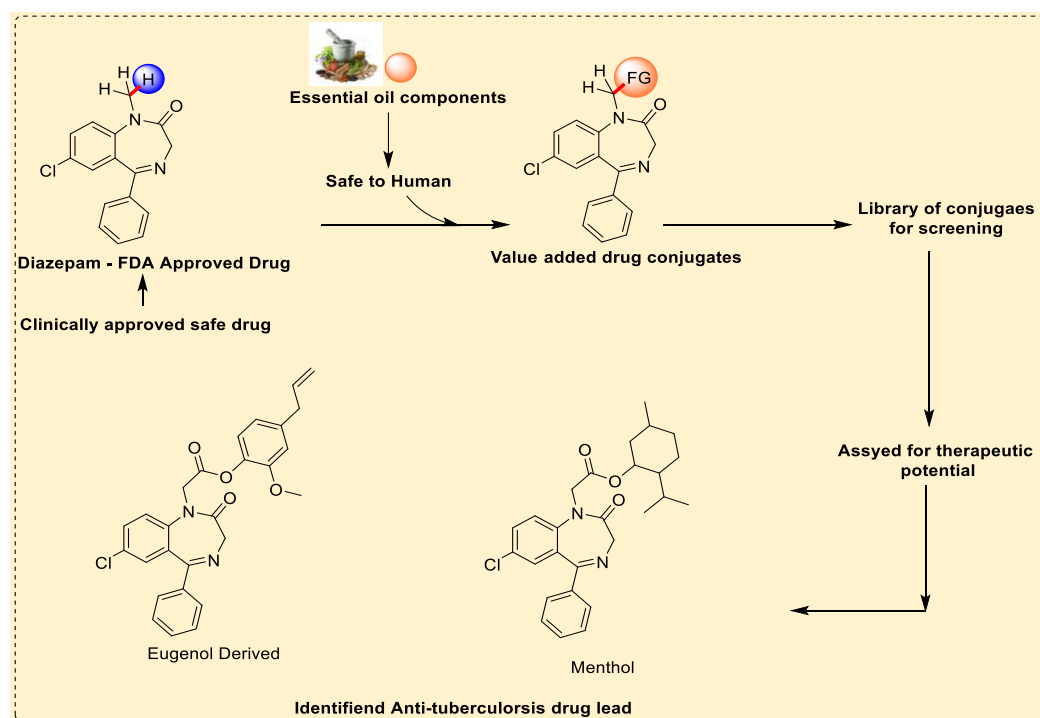
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Abstract

Benzodiazepines (BDZ), a known sedative and hypnotic compound¹ was assayed for functional derivatization and resulting medicinal properties, using a ligand library of aroma products obtain from aroma mission initiative of CSIR. BDZ was acidified at N₁ position and then EDAC coupled² with natural products (NP) such as Menthol, Eugenol, and Patchouli alcohol etc. Thus obtained NP-BDZ conjugates were *in-silico* investigated for therapeutic potential against different diseases causing protein targets. Network pharmacology server was used for target identification and find 189 different potential disease causing biological factors as primary hits. Primary docking based lead identification studies with BDZ showed almost comparable efficacy against tuberculosis when compared to reference commercial product (4TZK Ligand, $\Delta E = -0.193$). Further lead optimization studies using NP-BDZ conjugation and lead validation using Schrodinger, identified eugenol-BDZ and menthol-BDZ conjugate as potential anti-tuberculosis compounds. The identified NP-BDZ conjugates show better therapeutic potential than the chosen commercial reference and hold promise as a potent future drug, and demand further product characterization, formulation and clinical testing.



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Designing Highly Tunable Bioinspired Peptide Based Supramolecular Hydrogels via Non-Equilibrium Self-Assembly to Mimic the Differential Cellular Microenvironment

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Abstract

Peptide-based supramolecular systems aim to emulate the abilities of life forms by utilizing conserved sets of building blocks and chemical reactions to achieve diverse functionalities. Short-peptide-inspired nanomaterials, exhibiting properties such as self-assembly, recognition, catalysis, and actuation, have facilitated the formation of multifunctional nanostructures. In this context, we discuss the supramolecular design of short peptides derived from diverse proteins of Extracellular Matrix (ECM) by controlling the self-assembly pathways using a solvent-mediated approach. We explored two bio-inspired hydrogel scaffolds based on laminin as a minimalistic building block, where the self-assembly was triggered by solvent-switch method at different concentrations of DMSO (2% and 5%) respectively, to develop a dynamic supramolecular complex. Further, the close association of the laminin with other proteins of the basement membrane elevated our curiosity to explore the short peptide sequence of one of the bridging components of ECM i.e., Entactin. The novel tetrapeptide sequence adapted from the G3 domain of the entactin protein, based on the aromatic π - π interaction was capable of exhibiting three-dimensional nanofibrillar structures with distinct physical, mechanical, and biological activities at the nanoscale level. The versatility of functional supramolecular peptide architecture can offer an innovative approach for the development of cell-instructive scaffold.

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Unveiling Unique Photoluminescence and AIE Properties through the Brownian Rotor Embedded Fluorogenic Probe

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Abstract

Molecular rotors/motors are dynamic systems generally comprising rotor and stator parts. A specially designed Brownian rotor (BR) can exploit the thermal noises in the environment to perform rotational movement.¹ Previously, we have exploited Brownian rotational motion in the molecule to develop a power stroke module integrated motor for accessing thermal energy and conversion to electrical power. Such motors have potential applications in biomedical, energy harvesting^{2,3}, etc. Herein, we investigate the effect of Brownian rotors through the structural modulation of fluorogenic probes and the corresponding impact on the photoemissions. Our new system unraveled unique photoluminescence and aggregation-induced emission (AIE) in two binary solvent systems, DMF/water, and THF/water.⁴ Thus, in combination, AIE and BR in a single molecule can generate synergistic effects that lead to tunable optical properties. This exploration focuses on the interplay of the mechanical paddling action of a rotor and evolving fluorescence characteristics in the molecular system. Such molecules can be harnessed for various applications⁵ in biophysics, biochemistry, materials science, etc.. Along with its mechanochromic properties, we also demonstrate the unique temperature-induced AIE properties that manifested a hyperchromic effect and a hypsochromic shift caused by the rotor's mechanical paddling action.

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Functionalized Graphene Quantum Dot appended with Amphotericin B as a Novel Treatment Option for Visceral Leishmaniasis

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Abstract

This research explores the synthesis and characterization of Graphene Quantum Dots (GQDs) functionalized with Amphotericin-B (AmB) for treating Visceral Leishmaniasis, caused by *Leishmania donovani* amastigotes infecting macrophages. GQDs were synthesized from bioactive compounds extracted from mango leaves, followed by a series of processes including ethanol soaking, centrifugation, drying, and microwave heating. To facilitate AmB binding, GQDs were functionalized with L-cysteine, introducing amine groups. AmB was then mixed with the functionalized GQDs in dimethyl sulfoxide (DMSO) and sonicated to enhance attachment. Unbound AmB was removed through centrifugation, yielding drug-loaded GQDs. Characterization using UV-Vis spectroscopy, FTIR, SEM and TEM confirmed successful functionalization and structural integrity. The study assessed intracellular uptake of GQD-AmB in J774.A1 macrophage cells, revealing effective internalization and a significant reduction in parasite burden with minimal cytotoxicity compared to conventional treatments. Notably, the IC₅₀ of GQD-AmB was significantly lower than the CC₅₀, highlighting its potential as a cost-effective and safer therapeutic option for visceral leishmaniasis. These findings underscore the promise of novel nanomaterials in enhancing drug delivery and efficacy against parasitic infections.

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Solvation of Amino Acids and Related Thermochemical Behaviour in Presence of Univalent Electrolytes in Aqueous Medium

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Abstract

Solubility and associated thermodynamic parameters are extremely important for designing the mode of crystallization and separation of an amino acid from a mixture of amino acids and other biomolecules. The knowledge of solubility is also vital in chemical, chemical engineering, food and pharmaceutical concerns. The use of electrolytic ions might have a potential significance for the separation of biomolecules. Thus, designing most ordered crystallization and separation process of amino acid molecules necessitate knowledge on equilibrium-saturated solubility of these molecules in the presence of electrolytic salts.

From these points of view in this study, we measured the saturated solubility of glycine, DL-alanine, DL-valine, and DL-serine, L-Histidine, L-Proline in aqueous sodium and potassium iodide/chloride mixtures by formol titration. In this study, we also calculated the various physicochemical factors that are helpful in scheming the solubility and solvation energetics. The solvation thermodynamic data like free energy of transfer of the amino acids were also evaluated that can help to predict the possible stability of different conformations of the biomolecules like amino acids, peptides, as well as proteins.

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Catalytic Nanoprobes for Biofilm Eradication, Drug-delivery and Bioimaging

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Abstract

Designing and synthesizing catalytic nanostructures and fine-controlling their properties can be highly useful for biomedical and healthcare applications. We synthesized mixed-FeCo-oxide-based surface-textured nanostructures (MTex) as highly efficient magneto-catalytic platforms.^[1] MTex can produce defensive reactive oxygen species (ROS) over a broad pH range and effectively diffuse into the biofilm. MTex proved to be highly advantageous over the existing antimicrobials. In another example, we synthesized Au/Pt-based Janus nanostructures, like “egg-in-nest” morphology (Au/Pt-ENs) demonstrating as catalytic glucose-fueled autonomously motile drug-delivery platform.^[2] We implemented a new ‘dynamic-casting approach’ using silica yolk-shell cast providing the anisotropically confined concave hollow nanospace to grow curved Pt-dendritic porous networks. Au/Pt-ENs showed enhanced motion due to dual enzyme catalytic cascade at Au-Pt interfacial site, and in turn, showing molecular-laden transport to living cells. As a key catalytic-motile feature, high diffusiophoresis in cell culture media increased the nanomotor-membrane interaction events and facilitated cell internalization. Ascertaining the locations of nanostructures inside cell by their innate bioimaging modality would be highly advantageous. In this regard, silica-derived silicon (Si) is useful due to its high biocompatibility, stability, and photoluminescence. We synthesized hydrophilic Si-nanoshells encapsulated with catalytic PdNCs in a rattle-like configuration.^[3] Due to small size and hydrophilicity, these nanoprobes were easily endocytosed inside cells, demonstrating high biocompatibility and photostable Si-characteristic PL-based live cell-imaging. Intracellular Si-nanoprobes demonstrated excellent catalysis to synthesize bioimaging molecules.^[4-5]

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Modulation of Mechanical Properties of Low Molecular Weight Supramolecular Hydrogels of Calcium Cholate by Drugs of Varying Hydrophobicity: Effect on Drug Release, Antioxidant, and Antibacterial Properties

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Abstract

Bile salt based low-molecular-weight supramolecular hydrogels (LMWSH) serve as an appealing framework for drug delivery applications, owing to their natural origin, biocompatibility, and the peculiar distribution of hydrophobic and hydrophilic domains. In this work, LMWSH based on an ionotropic gel of sodium cholate assisted by Ca^{2+} ions (CaC) was developed as a drug delivery system for both hydrophilic and hydrophobic drugs. Diosgenin, Quercetin, Rutin, and Amygdalin were chosen as model drugs, having varying hydrophobicity. The mechanical strength of the CaC hydrogel is enhanced by increasing the hydrophobicity of the loaded drug. The close-knit mesh design of CaC hydrogels loaded with hydrophobic drugs resulted in controlled drug release compared to the hydrophilic drugs. Drug-loaded CaC hydrogels exhibited good swelling and thixotropy, making them suitable for injectable formulations. In kinetic drug release, both relaxation and diffusion mechanisms play a pivotal role. The antioxidant and antibacterial activity of the loaded drugs increased synergistically in the hydrogels. Thus, due to these properties, the hydrogels can be safely used as topical gels against wound healing. This study shows that bile salts exhibit potential to enhance the delivery of both hydrophobic and hydrophilic drugs, making them promising candidates for biomedical applications.

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Cyclodextrin Modified Biocompatible Chitosan-Cinnamaldehyde Schiff Base Hydrogels: Their Antibacterial, Antioxidant and Drug Delivery Potential

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Abstract

Designing biopolymeric hydrogels for optimal drug loading and release is crucial for advancing. In this work, we synthesized chitosan (CS) based hydrogels by initially cross-linked chitosan (CS) with cinnamaldehyde (CA) through a Schiff base reaction creating CSCA hydrogel. To address the stability issues of CA, it was encapsulated within γ -CD (CD) then combined with CS to form stable CSCDCA hydrogel system. Both hydrogels CSCA and CSCDCA were characterized in terms of their swelling behavior, water retention, FT-IR, SEM, rheology, antioxidant activity, antibacterial property, and cytotoxicity. CSCDCA showed much better swelling/water retention ratio, antibacterial activity and biocompatibility compared to CSCA hydrogels due to hydrophilic nature of CD. However, CSCDCA hydrogel exhibited slightly reduced mechanical strength compared to the CSCA hydrogels. Uptake and release kinetics of Rifampicin (Rif) by the CSCDCA hydrogels slightly decreased compared to CSCA hydrogels. The drug release in phosphate buffer saline (PBS) at pH 7.4 and 37 °C showed that more than 50 % of Rif was released within 24 h, by both the hydrogels following a Fickian diffusion mechanism. The release was pH dependent indicating their potential as pH responsive drug delivery system. These hydrogels demonstrate promise for sustained drug release and improved therapeutic outcomes in biomedical applications

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Engineering Microbe-Material Interface to produce Solar Chemicals and Fuels from CO₂.

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Abstract

Photosynthetic biohybrid systems combining light harvesting materials with microbial biocatalysts is a promising approach for sustainable synthesis of chemicals from CO₂. We have been demonstrating this through the process called microbial photosynthesis. This happens by bacteria hacking the photochemical activity of the light absorbing semiconductor, that's by capturing the reducing equivalents after photoexcitation to undergo microbe's metabolism converting CO₂ into value added chemicals and fuels. Nanocomposite metal chalcogenides and organic semiconductors are two class materials we have been utilizing for developing biohybrids.

On Integrating Cu₂ZnSnS₄ nanoparticles with bacterium called *Sporomusa ovata*, the biohybrid has converted CO₂ into valuable feedstocks such as acetate and ethanol with appreciable yield and quantum efficiency. Similarly, on hybridizing a linear poly (phenylic) organic semiconductor with a methanogenic archaeon, we have been successful in demonstrating a photo reforming process simultaneous with microbial photosynthesis doing an overall CO₂ to methane reduction reaction coupled with benzyl alcohol to benzaldehyde oxidation. A photocatalysis ecosystem engineering strategy called division of labour is also employed by co-culturing with an electron transport specialist bacteria for enhanced photosynthesis.

We are also Investigating the enigmatic electron transfer mechanism happening between the light absorber and microbe through time correlated Photoluminescence spectroscopy and Transient Absorption Spectroscopy.

RAFT Copolymerization of NVP and MA followed by Evaluation of their Thermoresponsive Properties

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Abstract

Poly(*N*-vinylpyrrolidone) (PNVP) has been utilized in a wide range of applications such as contact lenses, cosmetics, pharmaceutical tablets, wound and dental care, and as a plasma expander, based on its water solubility and biodegradability.¹ In contrast, poly(methyl acrylate) (PMA) is a hydrophobic polymer noted for its thermoresponsive behaviour.² Among the various controlled radical polymerizations, the reversible addition-fragmentation chain transfer (RAFT) process is the most frequently used technique to obtain functional polymers. However, for the RAFT method, the choice of a chain transfer agent (CTA) depends on the monomer chosen for polymerization. According to the literature, xanthates are utilized mostly for generating PNVP from the NVP monomer,³ and for active monomer MA trithioester CTA are used.⁴

In this work, our purpose is to synthesize copolymers from the NVP and MA monomers by the RAFT method to develop new polymers having both characteristics. For copolymerization, various CTAs are used. The kinetic investigation was carried out utilizing different CTAs, varied monomer input ratios, and initiator concentrations. Several copolymers were synthesized after optimization of reaction conditions and confirming the best CTA. Additionally, the polymer's thermoresponsive properties were investigated to see if it could be used for suitable biomedical applications.

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One-Pot Plasmonic Black Gold Nanoparticles for Efficient Photocatalytic CO Oxidation

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Abstract

"Black gold," is a distinctive plasmonic nanomaterial^{1,2} capable of absorbing a broad range of light, from visible to near-infrared wavelengths.³ It has shown exceptional performance in CO₂ reduction, alcohol oxidation, and seawater purification.⁴⁻⁶ However, its primary limitation lies in its complex multi-step synthesis process, which involves the gradual growth of Au nanoparticles over several days on dendritic fibrous nanosilica (DFNS) support.^{3,7-11} Furthermore, the need for solid separation through centrifugation after each cycle is an additional bottleneck.³

In this work, we explored a simplified and efficient one-pot synthesis method for producing plasmonic black gold.¹² This approach streamlined the process, reducing the synthesis time from days to hours and eliminating the need for solid separation, thus improving sustainability. Furthermore, DPC-60, synthesized using the one-pot method, demonstrated efficient catalytic performance in CO oxidation under light, achieving 87 % CO conversion at 4.0 W cm⁻² without external heating. *In situ* DRIFTS studies identified key adsorption sites for CO oxidation, revealing that bridged CO adsorbed on Au⁰ sites reacts more quickly than linearly adsorbed CO, with CO on high-coordinated Au⁰ sites exhibiting a faster reaction rate than on low-coordinated ones. This one-pot synthesis method accelerates the exploration of black gold's applications across various fields and opens the door to scalable industrial deployment.¹²

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Studying the Effect of Oxygen on Hydrogen Production from Formic Acid using Pd Alloy Catalysts

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Abstract

Formic acid (FA) dehydrogenation is a promising method for efficient hydrogen (H_2) production. Transition metal catalysts that selectively oxidize carbon monoxide formed during the FA dehydrogenation over H_2 in the presence of oxygen (O_2) are preferred. In this work, we examine the reactivity of Pd-ZnO towards H_2 production in the presence of O_2 from FA reaction. Pd-ZnO is synthesized by the ascorbic acid-assisted reaction method and the FA reaction is carried out in a temperature-controlled batch reactor at ambient pressures. H_2 production is analyzed through gas chromatography. Pd-ZnO provides H_2 turnover frequency (TOF) of $0.55 \text{ (mol } H_2) \cdot (\text{mol of Pd} \cdot h)^{-1}$, and selectivity is 8.69 % with 1 M FA at 298 K, whereas H_2 TOF is $2.74 \text{ (mol } H_2) \cdot (\text{mol of Pd} \cdot h)^{-1}$ and selectivity is 84% at 323 K. However, an increase in FA concentration to 2.75 M at 323 K results in negligible H_2 production from FA reaction. The absence of O_2 in the reaction environment increases the H_2 TOF by ~ 30 times to $20 \text{ (mol } H_2) \cdot (\text{mol of Pd} \cdot h)^{-1}$ and selectivity is 81.87 % from 1 M FA at 298 K. These findings are significant and open a promising direction for the influence of O_2 on the H_2 production from renewably sourced FA.

Keywords: Heterogeneous Catalysis, Hydrogen, Formic acid, Oxygen, Mechanism

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Microenvironment Effects from First-Principles Multiscale Modelling of Electrochemical CO₂ Reduction

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Abstract

Electrochemical CO₂ reduction (eCO₂R) is a promising route to achieve net-zero emissions, but optimizing electrode/electrolyte interfaces remains challenging. Along with catalyst design, electrolyte microenvironments, especially cations, play a crucial role in improving Faradaic efficiency [1,2]. However, tools for optimizing electrolyte effects are lacking due to complex interplay between surface kinetics and transport processes [3]. In this work, we develop an ab-initio multiscale model coupling DFT-derived microkinetics with a continuum-scale transport model to study eCO₂R on Ag surfaces for both liquid electrolytes and ionomers [4]. By explicitly accounting for the cations across all scales, the current density trends across different cation buffer identities align with experiments. Low concentration buffers show a favorable trade-off between Faradaic efficiencies and carbonate precipitation, showing optimal performance. Further, we observe a volcano dependence for current densities as a function of buffer concentrations, due to the inverse relationship between concentration of cations and CO₂ at the Outer Helmholtz Plane. The ionomers can break this dependence due to fixed charges on their backbones, however, water management becomes crucial to go towards high current densities. Overall, this study paves the way towards rational electrolyte design in eCO₂R.

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Continuous Flow Mediated Intramolecular Dehydrative Coupling for Macrocyclization using Heterogeneous Ni/Ru-Zeolite Catalyst

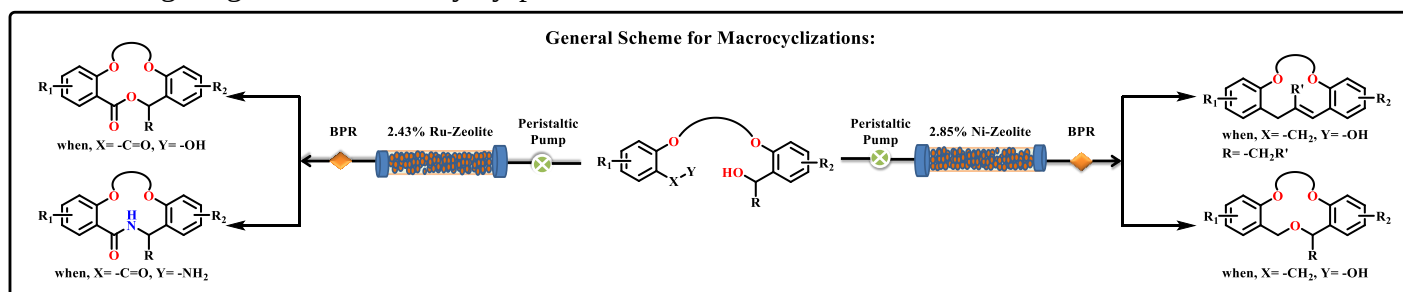
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Abstract

Continuous flow chemistry has invoked enormous attention over the last few decades and has created new opportunities in commercializing the products prepared in batch processes.¹ Based on the concept of green and sustainable chemistry, catalytic continuous flow reactions are fast, safe, reproducible, cost-effective, require less energy, and minimize waste.² Utilizing catalytic continuous-flow reactions, it is possible to construct complex molecules like macrocycles within a short reaction time. Macrocycles are large-sized cyclic structures constituting more than 12 atoms and are necessary scaffolds in medicines, materials, sensors, and natural products. Since macrocyclization is an entropically challenging process, it requires high-dilution conditions. Consequently, very limited heterogeneous catalyzed macrocyclization approaches are available. Thus, we have developed new protocols for synthesizing macrocycles in continuous-flow reactors using heterogeneous catalysts that provide high yields and selectivity. The initial study involves continuous-flow catalysis for synthesizing macrocyclic olefins³ and ethers⁴ using Ni-Zeolite through the intramolecular dehydrative coupling of diols. Next, we developed a reusable heterogeneous Ru-Zeolite catalyst for dehydrative macrocyclization, which afforded diverse range of macrocyclic lactones⁴ and lactams⁵ with different ring sizes. Ni/Ru-Zeolite as heterogeneous catalysts are cheap, highly reusable, and recoverable. Hence, this method is sustainable and atom economical giving water as the only by-product.



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Harnessing Plasmon-Enhanced Hot Electrons for Solar-Driven Catalysis in Black Gold-Nickel Systems

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Abstract

Conventional plasmonic nanocatalysts have intense light absorptions but are narrow.^{1,2} In this work, we have designed and synthesized dendritic plasmonic colloidosomes of Au (black gold)³, based “antenna reactor” of nickel that absorbs across the entire optical range.^{4,5} The plasmon-induced hot electrons and the intense electric field within the hotspots of black gold interact with reactants adsorbed on the Ni sites to activate the chemical bond. Black Gold-Ni exhibited exceptional performance in photocatalytic CO₂ hydrogenation, achieving a CO production rate of $2464 \pm 40 \text{ mmol g}_{\text{Ni}}^{-1} \text{ h}^{-1}$ with 95 % selectivity and was stable for over 100 h. The photocatalytic reaction showed a superlinear power law dependence on light intensity, and a higher kinetic isotope effect in light than that in the dark, affirming a hot-electron-mediated mechanism. Operando DRIFTS confirmed that CO₂ hydrogenation takes place via a direct dissociation pathway through linearly bonded Ni–CO intermediates.⁴ Additionally, the black gold-Ni catalyst was effective in catalyzing other challenging reactions like hydrodechlorination of dichloromethane and hydrogenation reactions.⁵ These findings suggest that the black gold-Ni “antenna-reactor” system holds significant potential for advancing plasmonic catalysis, particularly in the strategic reduction of CO₂ and other energy-intensive reactions under mild conditions using solar energy.

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Functionalized Graphene Derived Linear-Structure Single-Atom Gold(I) Catalyst for Dehydrogenative Coupling of Organosilanes with Alcohols

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Abstract

A strategy for the synthesis of gold-based single-atom catalyst (SAC) via one-step room temperature reduction of Au(III) salt and stabilization of selectively Au(I) ions on nitrile functionalized graphene (cyanographene, G-CN) is described. The graphene supported G(CN)-Au catalyst exhibits a unique linear structure of the Au(I) active catalytical sites promoting a multistep mode of action in dehydrogenative coupling of organosilanes with alcohols under mild reaction conditions as proved by advanced XPS, XAFS, XANES, and EPR techniques along with DFT calculations. The linear structure being perfectly accessible towards the reactant molecules, and the cyanographene induced charge transfer resulting in the exclusive Au(I) valence state, contribute to superior efficiency of the emerging two-dimensional SAC. The developed G(CN)-Au SAC represents, despite its low metal loading (ca.0.6wt %), the most efficient catalyst for the Si-H bond activation with turnover frequency up to 139494 h⁻¹ and high selectivities¹. Moreover, G(CN)-Au SAC can be easily prepared in multi-gram batch scale, works well towards for a continuous-flow mode.

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Shell Passivation in Perovskite Nanocrystals: Improving Stability and Optical Properties with Lead-Free $\text{Cs}_3\text{Bi}_2\text{Br}_9$ Coating

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Abstract

All-inorganic metal halide perovskites (ABX_3 , where $X = \text{Cl, Br, or I}$) hold significant promise for advanced optoelectronic devices. However, the extensive application of lead-based perovskites is hindered by their inherent toxicity and poor stability. One of the promising solutions is shell passivation using more stable material, lead-free $\text{Cs}_3\text{Bi}_2\text{Br}_9$ around CsPbBr_3 nanocrystals (NCs), forming $\text{CsPbBr}_3/\text{Cs}_3\text{Bi}_2\text{Br}_9$ core-shell nanocrystals. Here, we use the colloidal method for the epitaxial growth of lead-free CBB on CPB NCs. This approach not only shields the unstable components from environmental degradation but also offers a versatile method to fine-tune the material's optical properties. While this heterostructure fabrication results in the quenching of PL, optical measurements charge separation, as evident by transient absorption data. This Heterostructure provides a suitable option for photovoltaic application.

Monodispersed PdO Nanoparticles on the Surface of Polyaniline Nanotube and its Efficient Electrochemical Hydrogen Evolution

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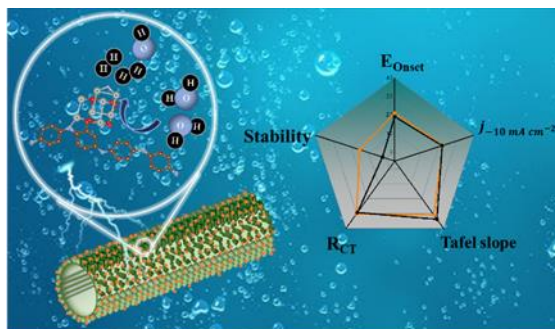
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Abstract

Spatially uniform as well as confined palladium oxide nanoparticles (PdO-NPs) are integrated selectively and uniformly on the surface of symmetrical organic acid doped polyaniline nanotubes (PANI_NTs) to generate a hybrid catalyst. Presence of amine sites provide uniform platform for PdO adsorption and electronic structure modification of active Pd sites resulting enhanced HER activity (only 67 mV overpotential to achieve 10 mA cm⁻² current density) and remarkable stability (15000 cycles) with negligible depletion in comparison to commercially available Pd/C catalyst.



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PANEL DISCUSSION-1 (16th December at 15:15 pm)



“Net Zero India: Nuclear, Solar, and CCU Solutions”

PANELIST:

Nuclear Energy in
Achieving Net-Zero



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Former Chairman,
Atomic Energy Commission

Green Hydrogen –
Fuel of the Future



Dr. ASHISH LELE
Director,
National Chemical Laboratory, Pune

CCU – Utilizing CO₂
for a Sustainable World



Dr. RAMAKRISHNA SONDE
Former Executive Director ,
NTPC Ltd.

Solar Energy as a Key
Driver for Net Zero



Prof. Prashant Kamat
University of Notre Dame, Indiana

Government Funding for
Research & Development



Dr. Neelima Alam
Associate Head, CEST, DST, GOI

MODERATORS:



Dr. Arun Kumar Nayak
Department of Atomic Energy (DAE), Mumbai



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TIFR, Mumbai



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BPCL, India



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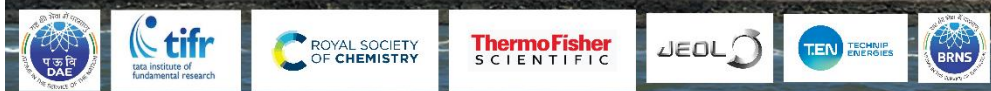
MODERATORS:



Prof. Gadi Rothenberg
University of Amsterdam, Netherlands



Prof. Vivek Polshettiwar
TIFR, Mumbai



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