

January 2024

CSI Communication

Monthly Newsletter of Catalysis Society of India

Circulated to all CSI Members

Important Announcement:

CSI newsletter shall be pleased to publish half a page write-up under the title, Centre of Excellence in Catalysis Research in India from any Indian Academics, Research laboratories or Industrial organizations. You may send your brief write-up on your research activities to us which will be published in coming issues of CSI.

You can also share your recent happy moments like publications, granted patents, technology commercialization, fellowship, awards, etc. to highlight in the CSI communication.

Energy Materials & Devices Group at IISc, Bangalore @ Dr. Sachin Rondiya

In the Department of Materials and Engineering at the Indian Institute of Science (IISc), **Dr. Sachin Rondiya** leads an independent research group comprising 15+ research students, including postdocs, PhD, MTech, and undergraduate students. His group is named 'Energy Materials and Devices,' reflecting the collective endeavor towards a singular aim: employing cutting-edge scientific approaches to develop highly efficient energy materials and devices. The group aims to address energy materials and device challenges through an engineering approach rather than relying solely on financial resources.

His group's primary research interests and experience lie in understanding & improving emerging material-based device performance. The research group focuses on engineering devices and conducting in-depth investigations of electronic properties of novel nanoscale semiconductor systems for a wide variety of applications, including but not limited to photovoltaics (PV), hydrogen production, and ultrafast photochemistry.

Their vision is to establish and pursue an ambitious interdisciplinary program of research, employing high-level experimental techniques to guide the rational design and synthesis of earth-abundant and cost-effective emerging next-generation materials for energy harvesting.

The research team comprises four distinct sub-groups that specialize in a diverse spectrum of fields, ranging from synthesis and fundamental studies to device fabrication.

Materials Design Group

The group is working on developing advanced nanomaterials for energy-efficient applications. They are dedicated to designing and synthesizing different materials, including chalcogen perovskites, chiral perovskites, and chalcogenide semiconductors. Chalcogen perovskites are known for their defect-



Kusuma Jagadish
IoE Postdoctoral Fellow
(Nov 2022-present)

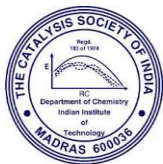


Durgesh Rambhau Borkar
JRF Research Scholar
(Aug 2022-present)



Shubha S Revanakar
Ph.D. Research Scholar
(Aug 2023-present)

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tolerant properties. However, synthesizing them in colloidal form at low temperatures is challenging. Therefore, the group is exploring different synthesis methods to produce them in their pure form. The team is also working on synthesizing chiral perovskite single crystals using the acid precipitation method and then analyzing the structural, optical, and morphological properties of these thin films. In addition, the group is working on synthesizing novel metal chalcogenide materials using the hot injection method.

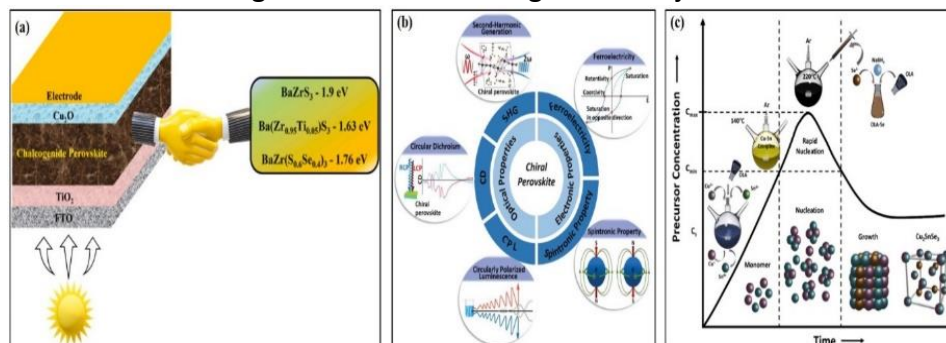


Figure 1. (a) Chalcogen Perovskites for solar cell DOI, (b) Chiral Perovskites DOI, and (c) Lamer Curve to understand the nucleation growth and mechanism

We study the Nucleation and Growth mechanism of ternary chalcogenides by the Lamer curve. Furthermore, we are investigating the band alignment and interface properties of heterojunctions to improve charge transport, reduce recombination, and enhance light absorption. To fully comprehend the potential of these materials, the team is focusing on understanding their properties, including the study of defect states. This comprehensive approach to materials science is critical for the successful development of nanomaterials that can be used to create more efficient energy solutions. With their expertise and dedication, the group is poised to make significant contributions to energy research.

Spectroscopy Group



Sangeetha C.K
PhD Research Scholar
January 2023 - Present



Sai Kumar
PhD Research Scholar
August 2022 - Present



Ganesh Rahane
PhD Research Scholar
January 2024 - Present



Swati Rahane
PhD Research Scholar
March 2021 - Present

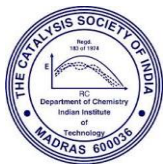


Animesh Mandal
Research Associate
May 2023 - Present

The spectroscopy group at Energy Materials and Devices Group focuses on charge carrier dynamics in perovskite and chalcogenide materials. Using advanced spectroscopic tools, they delve into exciton and polaron dynamics in perovskites like CsPbX_3 and study plasmonic structures in chalcogenides such as CuS , CTSe , CTSSe , and various perovskites. In the realm of chalcogenide materials, known for stability and non-toxicity, the group systematically explores composition and doping effects using optical spectroscopies. Techniques like transient absorption spectroscopy and photoelectron spectroscopy unravel trap states, recombination mechanisms, and electronic structures, particularly in materials like CuS , revealing intrinsic p-type behaviour and stoichiometry-dependent recombination mechanisms.

For 3D perovskite materials like CsPbX_3 , crucial for light-emitting devices, the group employs Transient Absorption Spectroscopy and Time-resolved TAS to decipher ultrafast carrier dynamics, providing insights into recombination and migration mechanisms. Extending their exploration to

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2D perovskite materials, the group utilizes Terahertz Spectroscopy and Time-resolved THz to probe low-energy excitations and carrier scattering processes. These studies shed light on quantum and dielectric confinement in 2D perovskite systems. Moreover, venturing into lead-free 3D $\text{Cs}_2\text{Ag}_x\text{Bi}_{(1-x)}\text{Cl}_6$ nanocrystals, the group tunes composition to achieve a direct band gap, resulting in nanocrystals with dual-colour emission and enhanced photoluminescence properties. This breakthrough opens avenues for high-performance lead-free perovskite optoelectronic devices, marking a significant stride in sustainable materials.

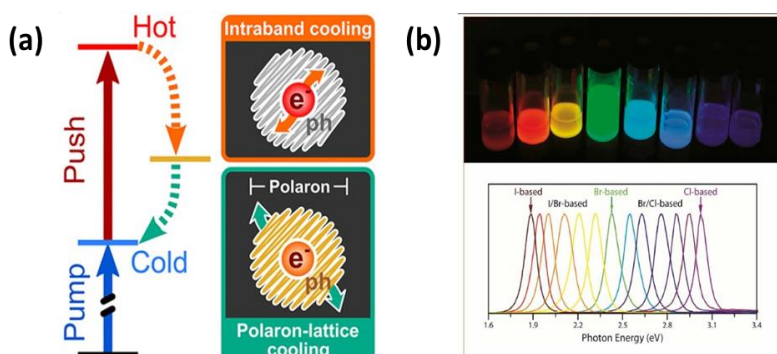


Figure 2. (a) Hot Polaron Photoconductivity Dynamics in Metal-Halide Perovskites ([DOI](#)), (b) Solutions of lead halide perovskite NCs of different halide composition under UV light illumination. By changing the halogen X in the material, it is possible to obtain bright emitters in the red–violet spectral range (top). Corresponding PL profiles (bottom)

Electrical Group

Our group is primarily focused on the comprehensive investigation of the electrical properties of materials that are synthesized within our laboratory. These include perovskites, chalcogenides, and chiral materials. In order to achieve a profound understanding of the behavior of

these materials, we employ a range of electrical characterization techniques, including deep-level transient spectroscopy (DLTS), impedance spectroscopy, electrochemical cyclic voltammetry, IV-CV measurements, and hall probe measurements. By utilizing these techniques, we aim to gain fundamental insights into the electrical properties of these materials. Our research endeavours are aimed at providing in-depth analyses of these materials, which will aid in furthering our understanding of their electrical properties. Deep-level transient spectroscopy allows us to study the energy levels within the materials, providing insights into charge carrier traps and their impact on electronic performance. Impedance spectroscopy helps us analyze the electrical response to varying frequencies, offering a comprehensive view of the material's electrical properties. Cyclic voltammetry helps in understanding the electrochemical behavior, providing crucial information about redox processes and charge storage capacities. The IV-CV measurements help in characterizing semiconductor devices by examining their current-voltage and capacitance-voltage relationships. Also, hall effect measurements allow us to determine critical parameters such as carrier concentration and mobility in a magnetic field.



Shatayu Deshpande
M.Tech
(Aug 2022 – Present)



Shambhavi Joshi
Ph.D. Scholar
(Aug 2023 – Present)



Hritwik Ghosh
Ph.D. Scholar
(Aug 2023 – Present)

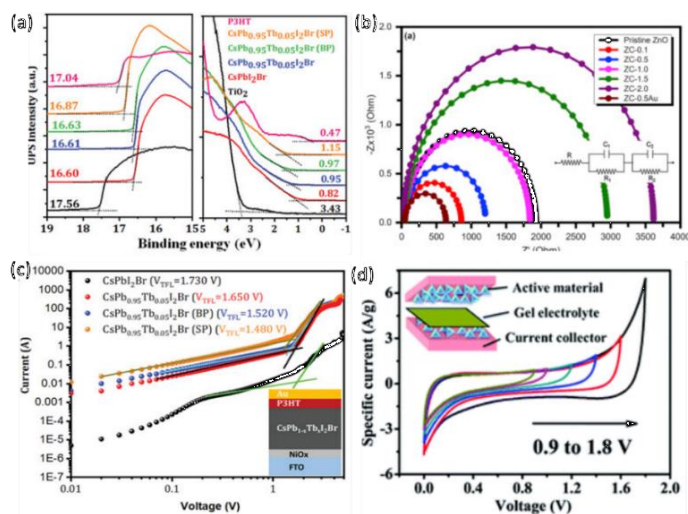


Figure 3. (a) Ultraviolet photoelectron spectra (UPS) of the TiO₂, CsPbI₂Br, CsPb_{0.95}Tb_{0.05}I₂Br, CsPb_{0.95}Tb_{0.05}I₂Br-(BP), and CsPb_{0.95}Tb_{0.05}I₂Br-(SP) and P3HT (DOI), (b) Electrochemical impedance spectroscopy (EIS) measurements of pristine ZnO, ZC, and ZC-0.5 Au thin films photoanodes in light (Nyquist plot), (c) Current density–voltage characteristics of single carrier (hole-only) of γ-CsPb_{0.95}Tb_{0.05}I₂Br-based devices (DOI), (d) CV curves of the flexible solid-state cell collected at a scan rate of 100 mV s⁻¹ scan rate in different voltage windows (DOI)

Our vision is to pave the way for possible breakthroughs in electronic devices and technologies, shaping the future landscape of materials science and electronics.

Photovoltaic Device Group

Within the laboratory, the Photovoltaic Device Group is working on enhancing the stability, durability, and efficiency of perovskite-based third-generation solar cells via exploring various avenues and novel techniques that can improve the structural, optical and electrical properties of the perovskite material and ultimately lead to enhancement of device performance. The group employs various approaches, mainly focusing on interface unravelling of 3D-2D halide perovskite heterostructures, incorporation of co-additives, and use of defect passivating agents to enhance the performance and propel the development of more robust and efficient solar cells.

Perovskite solar cells have shown great promise due to their cost-effectiveness and high efficiency, but they have faced challenges related to stability over time. The integration of 2D perovskite layers with 3D perovskite structures has proven to be a groundbreaking approach. Specifically, applying the 2D perovskite atop the 3D perovskite through post-treatment is anticipated to improve interface properties and subsequently lead to heightened stability. Furthermore, the inclusion of an organic spacer cation with diverse functional groups and varying chain lengths could potentially offer the desired properties for achieving highly stable and efficient PSCs. This design enhances the overall moisture and air stability of the solar cell, mitigating issues associated with degradation over time. The 2D-3D perovskite heterostructures not only bolster the solar cell's efficiency but also contribute to increased longevity, making them a key area of focus for the Photovoltaic Device Group.



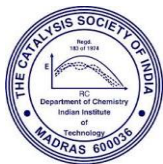
Dr. Nilesh Saykar
Postdoctoral Student
July 2023 – Present



Balpartap Singh
Ph.D. Student
Jan 2023 – Present



Dikshant Afria
Undergraduate Student
Mar 2023 – Present



Balpartap Singh, a second-year PhD student and a member of the Photovoltaic Device Group, focuses on employing cutting-edge experimental and spectroscopic techniques to pinpoint tailored interfaces with 3D-2D engineering to develop them into efficient thin-film photovoltaics processed at low temperatures using scalable methods.

Another significant avenue of research within the group involves the research efforts of Dikshant Afria, a senior undergraduate student; the research focuses on the development of high-efficiency perovskite absorber layers with enhanced morphology and charge transport capabilities.

The group is led by Postdoctoral student, Dr. Nilesh Saykar, whose work focuses on how passivating agents like EDAI_2 , pyridine, piperidinium, etc., passivate the surface defects and reduce the charge recombinations, resulting in longer charge carrier lifetimes and better charge separation. The agents act as a dopant to occupy monovalent cation vacancies in the perovskite lattice and induce a slow relaxation of the crystal strain, leading to an optimized crystal structure. These co-additives and defect-passivating agents play a crucial role in optimizing the film morphology of perovskite layers, improving the overall crystallinity, and reducing defects. This approach not only enhances the stability and durability of the solar cells but also leads to a notable increase in their efficiency. The meticulous selection and application of co-additives and passivating agents showcase the group's commitment to addressing real-world challenges in the field of perovskite-based solar technology.

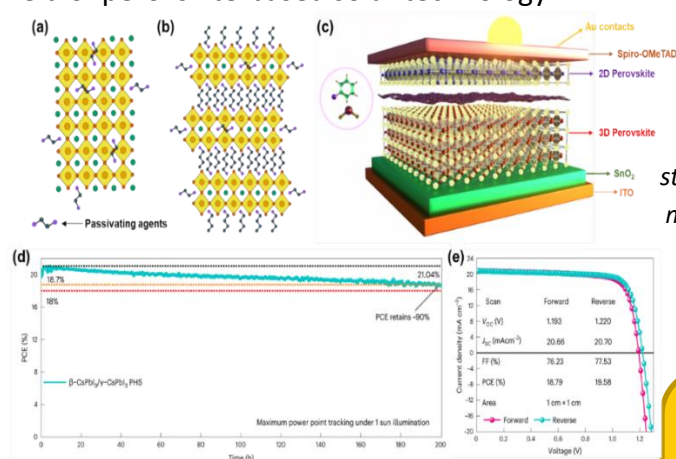


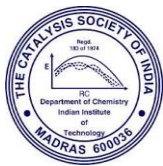
Figure 4. Structural reconstruction of (a) 3D Perovskite and (b) 2D Perovskite upon the addition of passivating agents enhancing their optical and structural properties, (c) Device architecture for 3D/2D multidimensional perovskite solar cells, (d,e) Performance of phase heterojunction perovskite solar cell reaching 21.5% efficiency (recently published in nature energy ([DOI](#)))

References

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- Shinde, P. et al. Plasmonic Au nanoparticles sensitized ZnO/CuO heterostructure for efficient photoelectrochemical water splitting. **International Journal of Hydrogen Energy** **54**, 1073–1084 (2024)
- Mali, S. S. et al. Phase-heterojunction all-inorganic perovskite solar cells surpassing 21.5% efficiency. **Nat Energy** **8**, 989–1001 (2023).

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Commercial & Policies

▪ **Novolooop and Aether Industries to Build New Pilot Plant for Circular Plastics**

Novolooop, a leading plastic circular economy technology company, has recently announced the construction of a pilot plant in India, marking a major milestone toward its vision of a truly circular world. This collaboration with Aether Industries, a publicly listed specialty chemical manufacturer and chemical process development provider, will demonstrate the scalability of Novolooop's Life cycling technology. This breakthrough technology transforms post-consumer plastic waste into monomers for the synthesis of virgin-quality, high-performance materials such as the company's Life cycled thermoplastic polyurethane.

Source: <https://www.process-worldwide.com/novolooop-aether-industries-to-build-new-pilot-plant-for-circular-plastics-a-370ace5f2dd1d4e8727f00e230828d84/>

▪ **BASF and Heraeus Precious Metals start up joint metal-recycling facility in China**

BASF Environmental Catalyst and Metal Solutions (ECMS) and Heraeus Precious Metals have commenced operations of a 50:50 joint venture facility, BASF HERAEUS Metal Resource Co., Ltd, (BHMR) in Pinghu, China. The facility recovers precious metals from spent automotive catalysts, enabling a circular economy. BHMR has a recycling capacity of approximately 10,000 tons of autocatalysts annually.

Source: <https://www.chemengonline.com/basf-and-heraeus-precious-metals-start-up-joint-metal-recycling-facility-in-china/>

▪ **India's First Cathode Active Material Manufacturer, Altmin Announces an Investment Outlay \$100 Million**

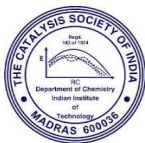
Hyderabad-based [Altmin](#), a cathode material manufacturer for lithium-ion batteries in India, has announced a plan to invest 100 million USD over the next five years. The company has secured growth capital from an Indian manufacturer of Iron Phosphate and other precursors to initiate a 3 GWh plant by 2025 for producing 9,000 tons of LFP annually. To support its CAM manufacturing operations, it has secured a tie-up with Bolivian state company YLB to source battery-grade lithium carbonate. Additionally, the company has forged a strategic collaboration with the [International Advanced Research Centre for Powder Metallurgy and New Materials](#) (ARCI) as its technology partner.

Source: <https://evreporter.com/altmin-aims-to-invest-usd-100m-in-cathode-material-manufacturing/>

▪ **GAIL and Trualt Bioenergy to set up CBG plants in India**

State-owned Gail India and Trualt Bioenergy will set up 10 compressed biogas (CBG) plants with an investment of more than USD 72 million. The two companies have entered into a joint venture agreement for setting up the plants. The proposed plants under the joint venture are expected to process over 600 million kilogrammes of organic waste like agricultural residue, sugarcane press

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<https://www.linkedin.com/groups/13923122/>*



mud, and spent wash -- waste generated during ethanol production to produce over 33 million kg of CBG, nearly 20 million kg of solid fermented organic manure and over 30 million kg of liquid fermented organic manure per annum. Each plant will have a capacity of 10,000 kg per day, resulting in a daily production of 100,000 kg of CBG.

- **Reliance ships first batch of certified circular polymers**

Reliance shipped its first batch of ISCC-Plus certified circular polymers, named CircuRepol (Polypropylene) and CircuRelene (Polyethylene). "RIL's commitment to sustainability is demonstrated through its innovative methods like chemical recycling which help create a Circular Economy. The company firmly believes in finding smart solutions to reduce plastic waste and inspire others to join in this journey towards a greener future," the release stated.

Source: <https://packagingsouthasia.com/she-safety-health-and-environment/sustainability-health/reliance-circular-polymer/>

- **Equinor and Linde to jointly develop 1GW blue hydrogen project in the Netherlands**

Norway's Equinor is planning to jointly develop a 1GW blue hydrogen project in the Netherlands with industrial gas firm Linde, shortly after Germany's state-owned gas company stated its ambition to buy 'giga-scale' volumes of blue H₂ from the Norwegian firm.

Source: <https://www.hydrogeninsight.com/production/equinor-and-linde-to-jointly-develop-1gw-blue-hydrogen-project-in-the-netherlands/2-1-1580246>

- **Oil India invites bids for 1 MW green hydrogen project in Himachal**

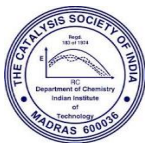
Oil India Limited (OIL) has issued a request for proposals to set up a 1 MW green hydrogen project. To be located in Himachal Pradesh, the project will have a generation capacity of 17 kg per hour. The unit should be engineered to operate for a minimum of 8,000 hours annually, running at full capacity.

Source: <https://renewablewatch.in/2023/12/26/oil-india-invites-bids-for-1-mw-green-hydrogen-project/>

Scientific Updates

- **Pt-doped Ru nanoparticles loaded on 'black gold' plasmonic nanoreactors as air stable reduction catalysts**

This study introduces a plasmonic reduction catalyst, stable only in the presence of air, achieved by integrating Pt-doped Ru nanoparticles on black gold. This innovative black gold/RuPt catalyst showcases good efficiency in acetylene semi-hydrogenation, attaining over 90% selectivity with an ethene production rate of 320 mmol g⁻¹ h⁻¹. Its stability, evident in 100 h of operation with continuous air flow, is attributed to the synergy of co-existing metal oxide and metal phases. The catalyst's stability is further enhanced by plasmon-mediated concurrent reduction and oxidation of the active sites. Finite-difference time-domain simulations reveal a five-fold electric field intensification near the RuPt nanoparticles, crucial for activating acetylene and hydrogen. Spectroscopic and in-situ Fourier transform infrared studies, combined with quantum chemical

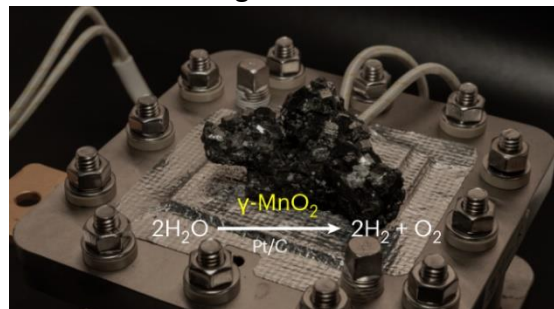


calculations, elucidate the molecular reaction mechanism, emphasizing the cooperative interaction between Ru and Pt in optimizing ethene production and selectivity.

Source: *Nature Communication* 15, 713 (2024). <https://doi.org/10.1038/s41467-024-44954-4>

■ Acid-stable manganese oxides for proton exchange membrane water electrolysis

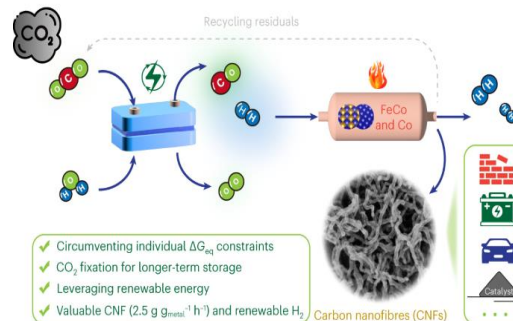
Authors report that optimizing the lattice oxygen structure of manganese oxide allows it to sustain the oxygen evolution reaction for over one month at $1,000 \text{ mA cm}^{-2}$ in $1 \text{ M H}_2\text{SO}_4$. The lifetime enhancement was achieved by substituting pyramidal oxygen with planar oxygen, which has a stronger Mn–O bond and thus suppresses the dissolution of manganese ions. Calculations show that the lattice oxygen dissolution is the bottleneck of deactivation, and this process is less favourable by over 0.2 eV on planar oxygen compared with pyramidal oxygen. Our material shows excellent performance even in a PEM electrolyser, reaching $2,000 \text{ mA cm}^{-2}$ at 2 V with durability exceeding $1,000 \text{ h}$ at 200 mA cm^{-2} . This study expands the potential of Earth-abundant catalysts for PEM electrolysis, which may mitigate the reliance on iridium.



Source: *Nature Catalysis*, 2024, <https://doi.org/10.1038/s41929-023-01091-3>

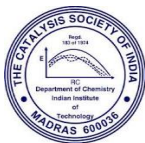
■ CO₂ fixation into carbon nanofibres using electrochemical–thermochemical tandem catalysis

Carbon dioxide fixation into value-added solid carbon such as carbon nanofibres (CNF) for longer-term storage represents a promising avenue for achieving net-negative carbon emissions. However, directly converting CO₂ to CNF via thermocatalytic approaches faces thermodynamic constraints, while electrocatalytic methods typically lead to amorphous carbon with limited yields or require energy-intensive conditions ($>720 \text{ }^\circ\text{C}$). An electrocatalytic–thermocatalytic tandem strategy for CNF production, which circumvents the aforementioned thermodynamic limitations by integrating the co-electrolysis of CO₂ and water into syngas (CO and H₂) with a subsequent thermochemical process at relatively mild conditions ($370\text{--}450 \text{ }^\circ\text{C}$, 1 atm), yielding CNF at a high production rate (average $2.5 \text{ g}_{\text{carbon}} \text{ g}_{\text{metals}}^{-1} \text{ h}^{-1}$) is presented. This tandem strategy opens a door to leverage renewable energy for decarbonizing CO₂ into valuable solid carbon products while producing renewable H₂.



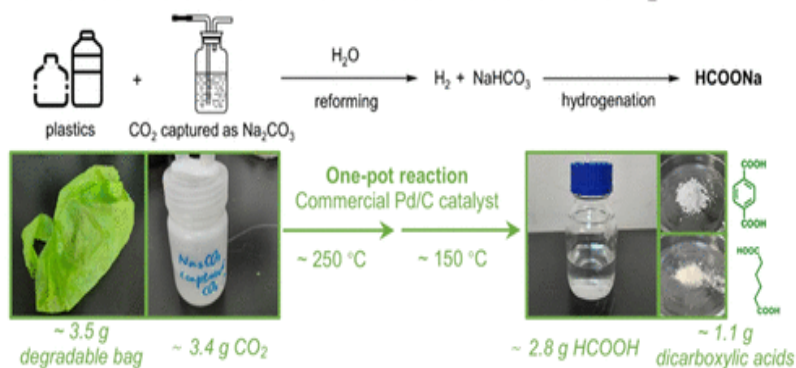
Source: *Nature Catalysis* 2024 <https://doi.org/10.1038/s41929-023-01085-1>

■ One-Pot Conversion of Polyester and Carbonate into Formate without External H₂



A one-pot, two-step catalytic process for transforming polyesters, such as poly(glycolic acid), carbonate, and water, into sodium formate with a high yield of 79%, using a commercial Pd/C catalyst is presented. This process involves the aqueous-phase reforming of polyester with water at 250–270 °C and

Two Wastes into One Chemical Process without External H₂



the hydrogenation of NaHCO₃ at 150 °C, utilizing H₂ generated during the reforming process. Notably, no external H₂ or other reactive reagents are required. This strategy can be applied for the co-conversion of poly(ethylene terephthalate) (PET), poly(butylene-adipate-co-terephthalate) (PBAT), and commercial biodegradable plastic bags with Na₂CO₃ obtained from CO₂ capture via a NaOH solution, opening up a new path for “turning trash into treasure”.

Source: *J. Am. Chem. Soc.* 2024, <https://doi.org/10.1021/jacs.3c12345>

Deep Insight into Characterizing the Metal–Support Interface in Heterogeneous Catalysis

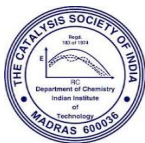
This Paper comprehensively summarizes the recent breakthroughs in characterizing metal–support interfaces in heterogeneous catalysts.

Source: *ACS Catalysis* 2024, <https://doi.org/10.1021/acscatal.3c04930>

Catalysis Research out of India

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3. J. H. Advani, A. Kumar, R. Srivastava, “Tailoring the Porosity and Active Sites in Silicoaluminophosphate Zeolites and Their Catalytic Applications” **Catalysis in Confined Frameworks: Synthesis, Characterization, and Applications**, 2024, 363-396 Wiley-VCH.
4. Ashish K Kar, Ganesh S More, Rajendra Srivastava, “Engineering the Porosity and Active Sites in Metal–Organic Framework” **Catalysis in Confined Frameworks: Synthesis, Characterization, and Applications**, 2024, 67-96 Wiley-VCH
5. Sphurti P Kulkarni, Amol A Kulkarni, “Continuous flow ozonolysis of cardanol for greener synthesis of bio-based monomers” **Journal of Flow Chemistry**, 2024 <https://doi.org/10.1007/s41981-024-00308-1>

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<https://www.linkedin.com/groups/13923122/>



6. Rajashri B Jundale, Bhagavatula LV Prasad, R Nandini Devi, Amol A Kulkarni, "Continuous Flow Synthesis of Mesoporous Silica Particles with Tunable Size and Structure" **Industrial & Engineering Chemistry Research**, 2024 <https://doi.org/10.1021/acs.iecr.3c03304>
7. Ranjit S Atapalkar, Amol A Kulkarni, "Batch and continuous flow mechanochemical synthesis of organic compounds including APIs" **Reaction Chemistry & Engineering**, 2024, 9, 10-25

Upcoming Symposium/Conferences/Seminars/Workshop

1. January 31-February 01, 2024-Future of Chemical Recycling 2024, Rotterdam, Netherlands
2. 18th International Congress on Catalysis from July 14-19, 2024, LYON, France.
3. XXIII International Symposium on Homogeneous Catalysis at Trieste, July 21-26, 2024
4. February 01-03, 2024-CGEC2024- The 1st International Congress on Green Environmental Catalysis, Osaka, Japan
5. March 06-08, 2024-EHEC 2024 -European Hydrogen Energy Conference, Bilbao, Spain
6. March 12-13, 2024-Chemical Recycling North America, Houston, TX, United States
7. International Conference on 'Emerging Trends in Catalysis & Synthesis 2024' from 07th to 09th March, 2024 at IIT, Kharagpur
8. "19th Edition of Global Conference on Catalysis, Chemical Engineering & Technology" at Rome, Italy, from September 19-21, 2024

Announcements

- CSI Congratulates the following CSI members on the recognition they received recently.

| Name | Achievements |
|--|---|
| <p>Dr. Raksh Vir Jasra, FNA, FNAE Senior Vice President & Head, Reliance Technology Group, Reliance Industries Ltd. Vadodara, & President, Catalysis Society of India</p>  | <p>ISAS Dr. Homi Bhabha Award 2023 will be conferral on 22nd Feb. 2024 at VNIT, Nagpur</p>  |

Quote of the Month

"Don't sit down and wait for the opportunities to come. Get up and make them."

—Madam C.J Walker

Editorial Team

Dr. Sharad Lande

Dr. Raksh Vir Jasra

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