Carbon Capture & Beyond

المعهد الهندي للتكنولوجيا دلهي أبوظبي

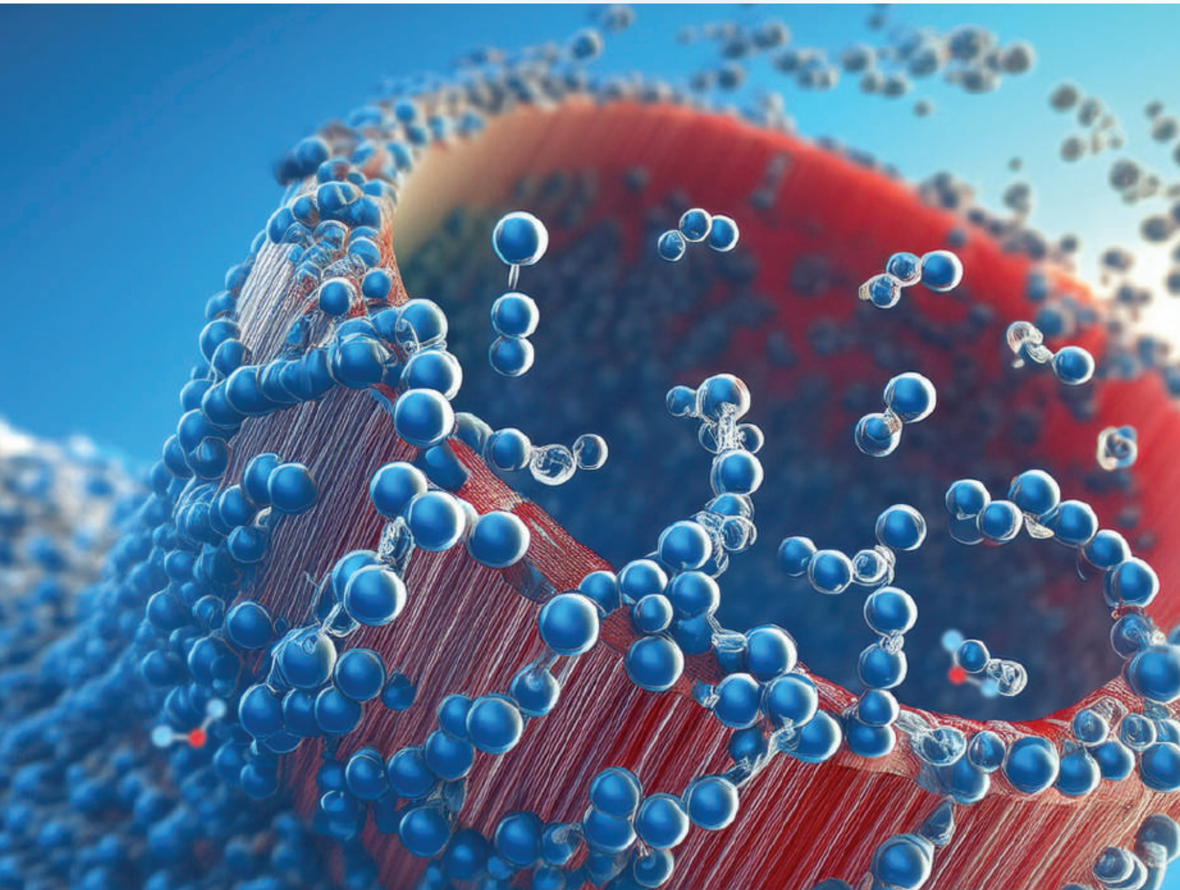
INDIAN INSTITUTE OF TECHNOLOGY DELHI ABU DHABI

International Workshop and Symposium on

Carbon Capture and Beyond (CCB)

Join the Global Dialogue on Decarbonization & Circular Economy Solutions

February 24 – 26, 2025 | IIT Delhi – Abu Dhabi



Preamble

Increasing carbon emissions pose an existential threat to life on Earth. To address this challenge, it is crucial to develop technologies that can effectively reduce CO_2 emissions by providing viable, near-term solutions. This requires thinking beyond traditional paradigms and adopting a multilevel perspective that fosters learning, experimentation, and breakthroughs in the energy technology landscape. By cultivating an environment conducive to innovation, disruptive changes are anticipated, paving the way for a desirable and sustainable energy transition.

IIT Delhi - Abu Dhabi is leading this effort by convening experts from both industry and academia for a three-day intensive workshop and research symposium focused on the future of carbon resources. The event will offer a multidisciplinary platform for researchers and professionals to explore cutting-edge advancements in decarbonization strategies, with a particular focus on molecular, process, and systems-level innovations. It aims to bridge the gap between fundamental research and industrial applications.

CCB Carbon Capture & Beyond

In addition to addressing key aspects of carbon capture, the workshop and symposium will highlight sustainability and circular economy principles by exploring the reutilization of captured carbon to create value-added products such as fuels, chemicals, and materials. Advanced technologies, including artificial intelligence (AI) and machine learning (ML), will also be examined as transformative tools to optimize and accelerate material discovery, enhance process efficiency, and enable systems-level integration.

Through these discussions, participants will gain valuable insights into how these technologies can work together to develop scalable and sustainable solutions for decarbonization.

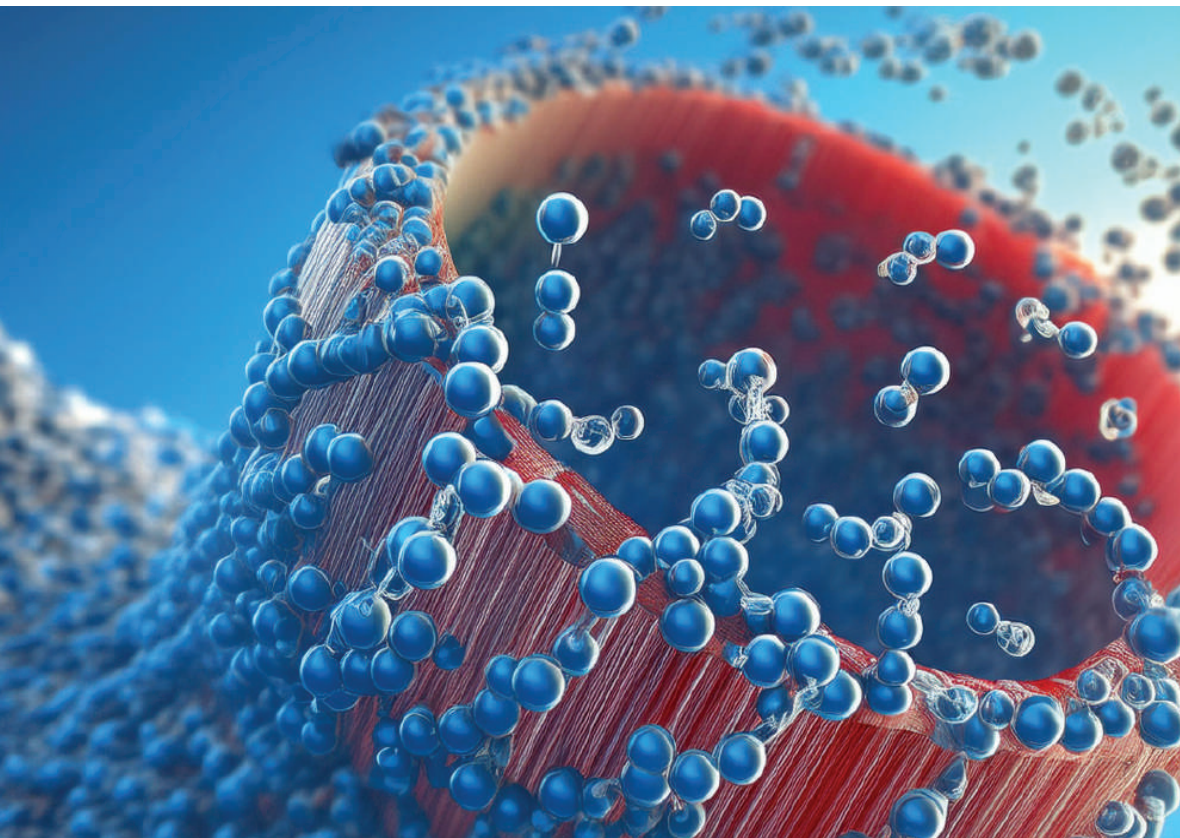
Key Areas of Focus

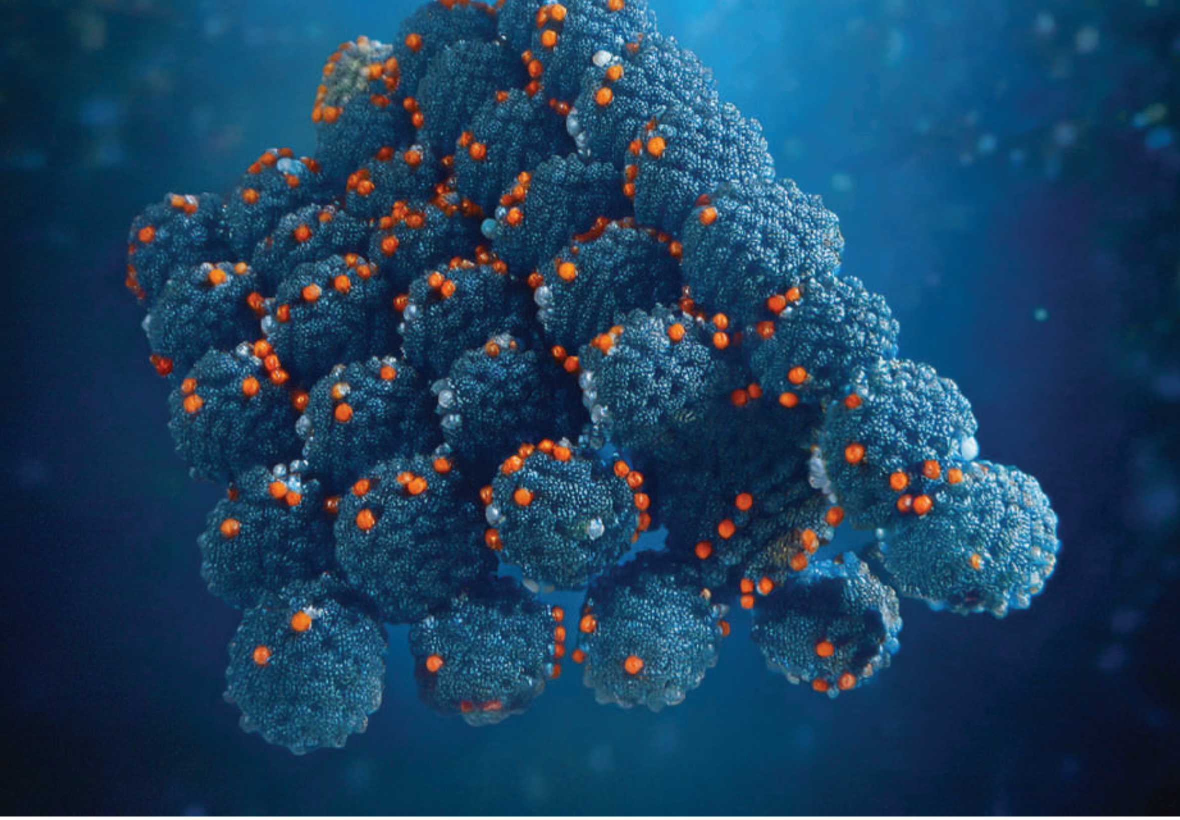
Carbon Capture
& Beyond

01

Fundamental Understanding of Molecular-Level Mechanisms

- Explore the design and performance of advanced materials, including metal-organic frameworks, zeolites, and membranes, for efficient CO_2 capture and storage.
- Discuss the role of molecular modeling, simulations, and AI-driven tools in optimizing material properties for adsorption and separation processes.





02

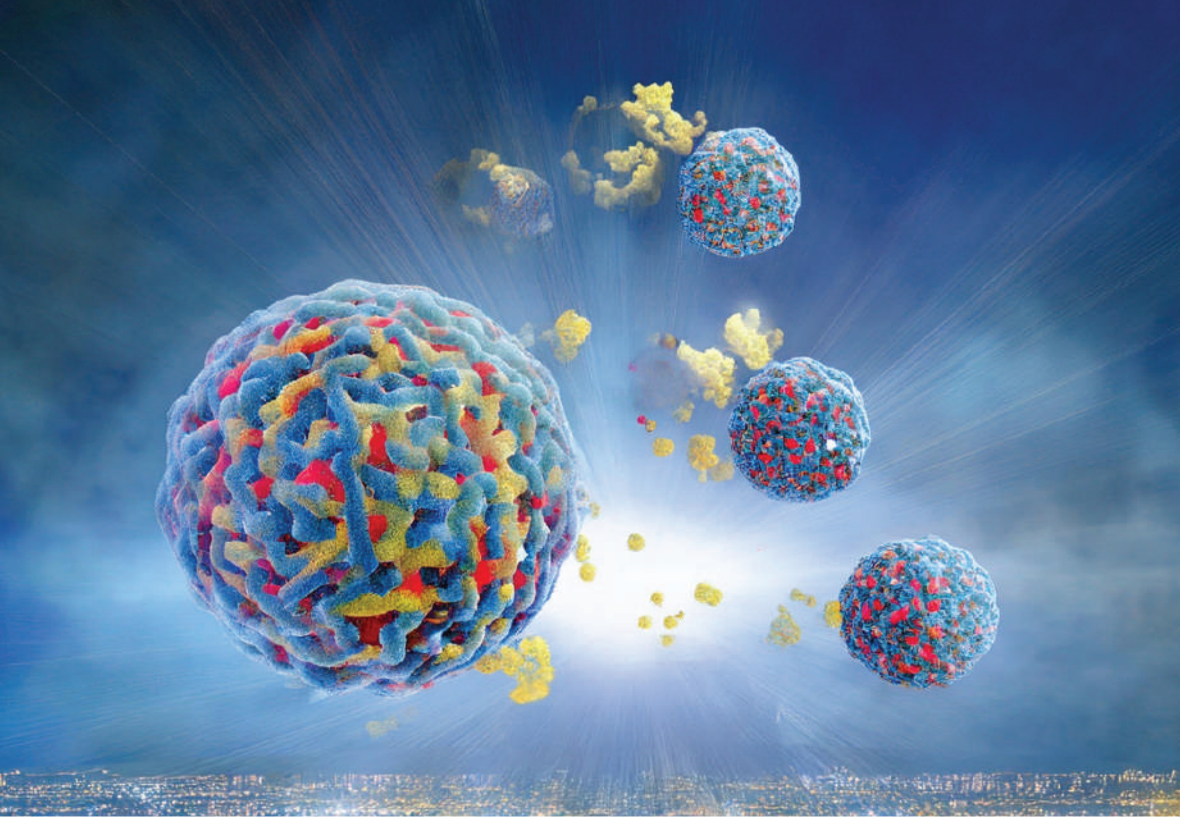
Process-Level Design and Optimization

- Analyze innovative process designs for carbon capture, such as chemical looping, post-combustion capture, and direct air capture systems.
- Investigate energy efficiency improvements and the integration of renewable energy sources into carbon capture processes to enhance sustainability.
- Highlight the application of AI for predictive modeling, process optimization, and real-time monitoring to maximize performance and improve efficiency.

03

Systems-Level Integration

- Assess the critical role of carbon capture within broader energy systems, encompassing power plants, industrial applications, and carbon utilization pathways.
- Examine techno-economic analyses, lifecycle assessments, and policy frameworks that support decarbonization efforts and ensure scalability.
- Utilize AI for complex systems modeling and decision-making to optimize the integration of carbon capture into energy and industrial systems.



04

Advancing Beyond Carbon Capture with Circularity

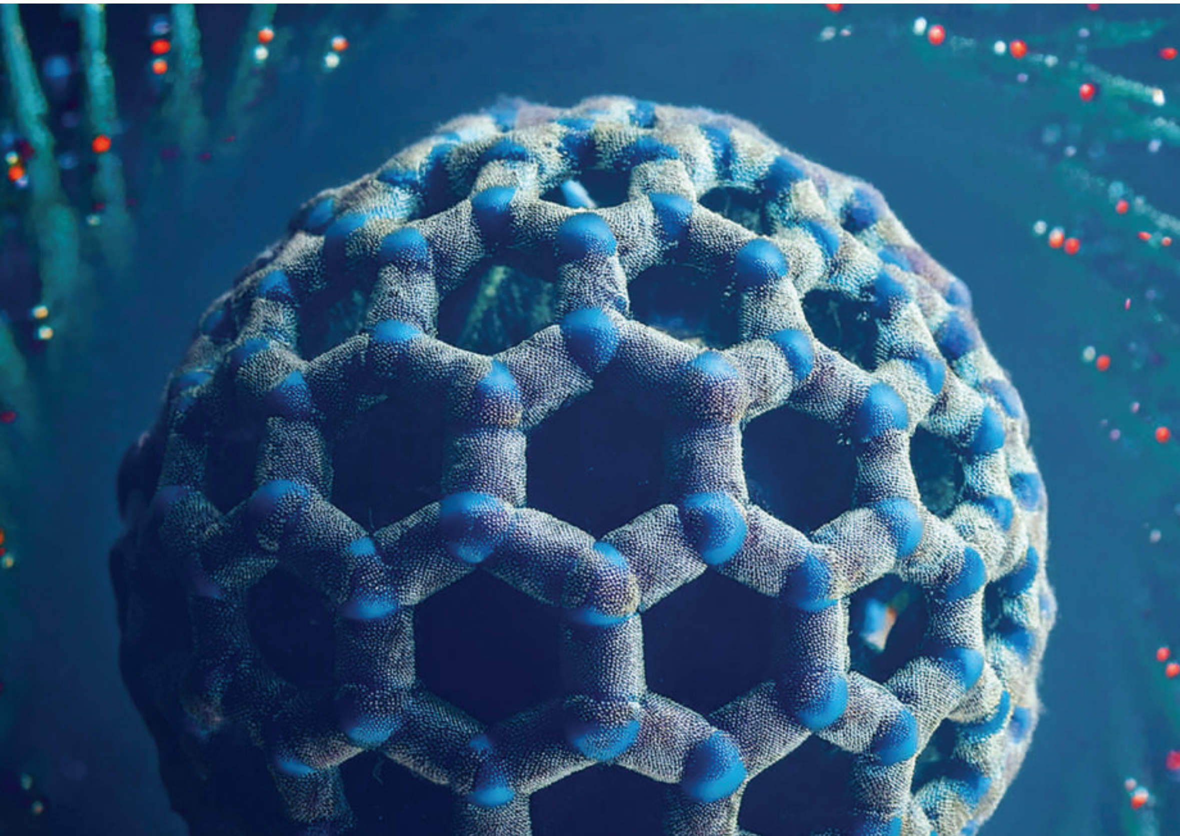
- Highlight innovative applications of captured CO_2 in producing sustainable fuels, chemicals, and materials, fostering a circular economy.

- Explore pathways to reduce waste and enhance resource efficiency through closed-loop systems that reutilize carbon in value-added processes.

- Leverage AI for designing circular workflows and maximizing the reuse and recycling of resources.

05 Fostering Interdisciplinary Collaboration

- Promote knowledge exchange among researchers, industry professionals, and policymakers to accelerate CCB technology development and deployment.
- Identify and initiate collaborative projects aimed at addressing global challenges in decarbonization, sustainability, and circular economy principles.



Program

24
25
26

February

February 24th

08:30 - 09:00	**Registration**	
09:00 – 09:10	**Welcome Note**	Prof. Shantanu Roy
	DAY 1: SESSION I	
09:10 – 09:30	**Challenges and Opportunities for Carbon Capture in the Transition to Net Zero**	Prof. Rangan Banerjee
09:30 – 10:10	**Materials and Processes for CCB**	Prof. Ahmed Al Hajaj
10:10 – 10:40	**Coffee Break**	
	DAY 1: SESSION II	
10:40 – 11:20	**Carbon Management in Hard to Abate Sectors**	Prof. Preeti Aghalayam
11:20 - 12:00	**Sustainability and Circularity in CCB**	Prof. Bhavik Bakshi
12:00 - 12:40	**Carbon Recycling for Sustainable Energy: A Journey from Fundamental Chemistry to Green Technologies**	Prof. Sebastian C. Peter
12:40 – 13:30	**Group Picture and Campus Tour**	
13:30 – 14:30	**Lunch Break**	
	DAY 1: SESSION III	
14:30 – 15:10	**Plasmonic Black Gold: A Catalyst for Solar-Driven CO_2 Conversion**	Prof. Vivek Polshettiwar
15:10 – 15:50	**High-throughput and AI Screening of Porous Materials for Biogas Purification**	Prof. Elena Besley
15:50 – 16:20	**Integration of CCU in a Coal-to-Methanol Pilot Plant: Bridging the Gap to Net Zero**	Prof. Divesh Bhatia
16:20 – 17:00	**Coffee Break**	
17:00 – 19:00	**Cultural Excursion**	

February 25th

	DAY 2: SESSION I	
09:00 – 09:30	**Open Framework Material Catalysts for CO_2 Utilization**	Prof. Dinesh Shetty
09:30 – 10:00	**Advanced Materials Characterization for Carbon Capture and Beyond: Use of AI and ML tools**	Dr. Rachit Khare
10:00 – 10:40	**Molecules to Processes: Ad Hoc Design of Materials for CO_2 Capture and Utilization by Multiscale Modeling**	Prof. Lourdes F. Vega
10:40 – 11:10	**Coffee Break**	
	DAY 2: SESSION II	
11:10 – 11:40	**Application of AI in CCB**	Prof. Hariprasad Kodamana
11:40 – 12:20	**Generative AI for Sustainability**	Dr. Alex Aliper
12:20 – 13:30	**Poster Session**	
13:30 – 14:30	**Lunch Break**	
	DAY 2: SESSION III	
14:30 – 15:30	**Panel Discussion: Opportunities for AI in CCB**	
15:30 – 16:00	**Advances in Reactor Design for CCB**	Prof. Sreedevi Upadhyayula
16:00 – 16:30	**Coffee Break**	
16:30 – 17:00	**Tuning the Physicochemical Attributes of Catalytically Active Materials for Better Understanding of Struture-Property-Performance Triad**	Prof. Manjesh Kumar
17:00 – 17:30	**Capture and Electrochemical Conversion of Carbon Dioxide**	Prof. Ahsanulhaq Qurashi
17:30 – 18:00	**Publishing and Reviewing for Nano Letters**	Prof. Elena Besley
18:00 – 18:30	**Group Photo**	
18:30 – 20:00	**Networking & Dinner**	

February 26th

	DAY 3: SESSION I	
09:00 – 09:30	**Strategic Approaches for CO_2 Emissions Reduction in Steel, Power and Transportation Industries**	Prof. Ejaz Ahmad
09:30 – 10:00	**The Art of Designing Multifunctional Catalysts for Value-Added Products: Fundamentals and Beyond**	Prof. Kyriaki Polychronopoulou
10:00 – 10:40	**New Industrial Approaches for CCB**	Dr. Mathew Aneke
10:40 – 11:30	**Poster Session and Coffee Break**	
	DAY 3: SESSION II	
11:30 – 12:10	**Three Stage CCUS Integration in Industrial Landscape: End of Pipe (EOP), CO_2 Compliant Designs (CCD), CCUS in One Pot (COP)**	Prof. R.R. Sonde
12:10 – 12:40	**Opportunities for Innovations in CCB: Developing a Multi-Level Perspective**	Prof. M. Ali Haider
12:40 –14:00	**Lunch Break**	
	DAY 3: SESSION III	
14:00 -14:30	**Decarbonizing Energy Storage and Utilization: Pathways for a Low-Carbon Future**	Prof. Dibakar Rakshit
14:30 -16:30	**Workshop and Focused Group Discussion**	
16:30 – 17:00	**Concluding Remarks and Awards**	

21+ Speakers

Speakers

Learn from the Pioneering Voices in Carbon Innovation and Sustainable Energy.

Challenges and Opportunities for Carbon Capture in the Transition to Net Zero

Prof. Rangan Banerjee

Indian Institute of Technology Delhi, India

Biosketch

Prof. Rangan Banerjee is currently the Director, IIT Delhi. From February 2022, he is on lien from IIT Bombay where he served as the Forbes Marshall Chair Professor in the Department of Energy Science and Engineering - a Department that he helped start in 2007. His areas of interest include energy management, modelling of energy systems, energy planning and policy, hydrogen energy and fuel cells.

Prof. Rangan Banerjee currently serves on the editorial board of International Journal of Sustainable Energy, International Journal of Sustainable Engineering, International Journal of Thermodynamics. He has been involved in setting up a megawatt scale Solar Thermal Power Testing, Simulation, Research Facility sponsored by the Ministry of New and Renewable Energy (MNRE) and is the faculty advisor of Team Shunya- India's first student team in the Solar Decathlon Europe finals. He has been involved in advising the city, state regulatory commission and energy agency, Niti Aayog, MNRE on energy issues and worked with several Indian and international industries.

Prof. Banerjee has been the Dean (R&D) and received the Excellence in Teaching Award from IIT Bombay and is a Fellow of the Indian National Academy of Engineering. Prof. Banerjee is also an Adjunct faculty (Honorary) in the Department of Engineering & Public Policy, Carnegie Mellon University.

Materials and Processes for Carbon Capture and Beyond

Prof. Ahmed Al Hajaj

Research & Innovation Center on CO_2 and Hydrogen, Department of Chemical & Petroleum Engineering, Khalifa University, Abu Dhabi, UAE

Abstract

Carbon capture and storage (CCS) is essential for achieving net-zero emissions, yet conventional materials and processes face challenges such as high energy consumption, degradation due to flue gas impurities, and efficiency losses. To enable large-scale deployment, novel materials and processes must enhance efficiency, reduce costs, and ensure high purity, recovery, and durability under real-world conditions. A major challenge is the lack of comprehensive performance data, hindering material selection and optimization. Addressing this requires research integration to compile, assess, and validate material properties, stability, and process performance at the enterprise level. This talk explores pathways to accelerate CO_2 capture through advanced processes including novel solvents and sorbents such as reactive materials from steel slag for calcium looping. By integrating experimental research with multiscale modelling and process optimization, we aim to improve capture kinetics, capacity, and efficiency, making CCS more viable and scalable.

Biosketch

Dr. Ahmed Al Hajaj is an Associate Professor of Chemical and Petroleum Engineering at Khalifa University and the theme lead for CO_2 utilization at the Research and Innovation Center for CO_2 and Hydrogen (RICH). Previously, he led the CO_2 capture and storage theme at the center. He was a visiting professor at MIT from 2015 to 2016. Dr. Al Hajaj holds a B.Sc. in Mechanical Engineering from the University of Arizona, two master's degrees—one in Mechanical Engineering from the University of Miami and another in Sustainable Energy Futures from Imperial College London—and a Ph.D. in Chemical Engineering from Imperial College London. His research integrates chemical engineering, operations research, computational chemistry, and biology, focusing on process systems engineering, product synthesis, optimization, and control. He aims to develop systematic tools to enhance industrial efficiency and sustainability, particularly in low-carbon technologies.

Carbon Management in Hard to Abate Sectors

Prof. Preeti Aghalayam

Indian Institute of Technology Madras
Zanzibar, Tanzania

Abstract

The increasing CO_2 emissions from industries such as cement, steel, and power generation represent a significant challenge to global sustainability. Addressing these challenges requires a dual approach: transitioning to non-fossil fuel-based power generation and effectively managing the CO_2 emissions already produced. In our laboratory, we have employed a mathematical modelling framework to explore critical aspects of CO_2 emissions and their potential utilization. Converting CO_2 into value-added chemicals, such as methanol, presents a promising solution. However, the feasibility and scalability of such approaches for the future remain uncertain. While the transition from coal to renewable energy is often seen as a necessary step, its implications for traditional industries like cement and steel are complex and require thorough evaluation. This presentation will critically assess various options, including green versus grey hydrogen, CO_2 sequestration versus chemical conversion, and the trade-offs between economic feasibility and environmental impact. Focusing on the context of India, this work provides model-based insights into viable pathways for reducing industrial CO_2 emissions while maintaining a balance between sustainability and economic growth.

Biosketch

Preeti Aghalayam is a Professor of Chemical Engineering at IIT Madras, specializing in automotive catalysis, underground coal gasification, and CO_2 utilization. She earned her BTech from IIT Madras (1995), MS from the University of Rochester (1996), and PhD from the University of Massachusetts Amherst (2000), followed by postdoctoral research at MIT. Previously, she was a faculty member at IIT Bombay. She has received the Amar Dye Chem and Young Achiever awards from IIChE and the INAE Young Engineer Award. Featured in 75 Women in STEAM by India's Principal Scientific Adviser, she was appointed Director-in-Charge of IIT Madras Zanzibar in 2023.

Sustainability and Circularity in Carbon Capture and Beyond

Prof. Bhavik Bakshi

School for Engineering of Matter, Transport and Energy, Arizona State University, USA

Abstract

Carbon capture, utilization, and storage (CCUS) are expected to play a pivotal role in achieving net-zero greenhouse gas emissions in the coming decades. However, the successful realization of this goal will require the integration of additional technologies, including the electrification of chemical processes, the adoption of circular economy strategies for chemical products, a heightened reliance on renewable energy, and the utilization of biomass. Moreover, economic policies, regulatory frameworks, and ecological solutions will be essential in guiding this transition.

This presentation explores recent advancements in systematic methodologies that facilitate this transition from economic, ecological, and societal perspectives. It emphasizes the development of open-access models for the chemicals and materials industry, the application of generative artificial intelligence to drive future innovation, and structured approaches for designing roadmaps that support sustainable transformation. Practical applications, such as the use of multilayer films in polymer products, will illustrate the implementation of these strategies.

Biosketch

Bhavik Bakshi holds the Wrigley Professorship at Arizona State University with appointments in the School for Engineering of Matter, Transport and Energy, School of Sustainability, and School of Complex Adaptive Systems. He is also an emeritus professor in Chemical and Biomolecular Engineering at The Ohio State University. His research develops systematic methods to ensure engineering supports a sustainable transformation, resulting in solutions that respect nature's limits, promote social justice, and drive economic prosperity. He has received recognitions from the Computing, Environmental, and Sustainability divisions of AIChE. He earned his Bachelor's in Chemical Engineering from the Institute of Chemical Technology, Mumbai, and an MS and Ph.D. in chemical engineering from MIT, with a minor in Technology and Environmental Policy at Harvard's Kennedy School of Government.

Carbon Recycling for Sustainable Energy: A Journey from Fundamental Chemistry to Green Technologies

Prof. Sebastian C. Peter

New Chemistry Unit and School of Advanced Materials, Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru, India

Abstract

Two of the most pressing scientific and technological challenges facing humanity today are energy and climate. Current energy production and utilization largely depend on the combustion of carbonaceous fuels such as coal, petroleum, and natural gas, which release CO_2 and disrupt Earth's carbon cycle. Approximately 30 billion tons of CO_2 are emitted annually from the burning of these fuels and from the industrial sector. If this CO_2 could be converted into valuable chemicals, it could significantly impact the global economy.

This talk highlights recent advancements in materials, including intermetallics, chalcogenides, oxides, and organic-inorganic hybrids, which serve as efficient catalysts for CO_2 conversion into chemicals and fuels. We are capturing CO_2 from industrial flue gases and converting it into value-added products such as methanol, CO, methane, dimethyl ether, and C_2–C_5 and C_5–C_{11} gasoline hydrocarbons.

Biosketch

Dr. Sebastian C. Peter received his PhD (chemistry) from the University of Münster, Germany (2006). He was a post-doctoral fellow at Max Plank Institute for Chemical Physics of Solids, Dresden, Germany (2006-07) and Northwestern University, USA (2007-10). Dr. Peter is currently the professor at New Chemistry Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore. His broad research interests include the development of solid-state inorganic materials for various applications ranging fuel cell, CO_2 reduction and hydrogen production. He has more than 240 peer reviewed publications and 12 patents. Dr. Peter is also part of the Editorial Advisory Board of JACS, Chemical Science, ChemSusChem and JSSC. He is the recipient of Swarna Jayanti fellowship and elected as the fellow of Indian Academy of Science.

Plasmonic Black Gold: A Catalyst for Solar-Driven CO_2 Conversion

Prof. Vivek Polshettiwar

Division of Chemical Sciences,
Tata Institute of Fundamental Research,
Mumbai, India

Abstract

Addressing the challenge of CO_2 utilization through advanced materials is crucial for a sustainable future. This talk will present research on Plasmonic Black Gold, an innovative catalyst that efficiently captures solar energy to convert CO_2 into valuable fuels and chemicals. By engineering gold into a black, highly light-absorbing form and integrating it with nickel, we have developed a catalyst capable of driving selective solar-powered CO_2 conversion into syngas with remarkable efficiency. This lecture will highlight the rationale behind its design, synthesis, and catalytic performance, emphasizing the role of plasmonic effects, nanoscale engineering, and strong metal-support interactions. Insights from in situ spectroscopic techniques provide a deeper understanding of reaction pathways, shedding light on the fundamental processes enabling efficient CO_2 activation and conversion. Beyond CO_2 reduction, this system has potential applications in other solar-driven catalytic transformations, demonstrating how functional nanomaterials can contribute to a carbon-neutral future.

Biosketch

Vivek Polshettiwar is a professor of chemistry at TIFR, Mumbai. His research focuses on advanced nanomaterials and nanocatalysis for harvesting solar energy and converting CO2 into valuable chemicals and fuels. He has published nearly 150 articles and also filed 12 national and international patents. He is the recipient of the prestigious ORISE Research Fellowship at US-EPA. He is Fellow of National Academy of Sciences, India; Indian Academy of Sciences and Royal Society of Chemistry, UK. He received the 2022 IUPAC-CHEMRAWN VII prize for green chemistry and the Falling Walls Award in Physical Sciences-Top 10. In 2024, he was awarded the Shanti Swarup Bhatnagar (SSB) Award, the highest and most prestigious award given in the area of science in India, by the President of India.

High-throughput and AI Screening of Porous Materials for Biogas Purification

Prof. Elena Besley

School of Chemistry,
University of Nottingham, UK

Abstract

Biomethane derived from biogas can serve as a valuable source for energy storage and transport applications. Primarily composed of CH_4, biogas also contains significant amounts of CO_2 and trace gases. Effective purification methods are essential to remove these impurities and enhance the calorific content of the gas. While conventional techniques can achieve biomethane purity levels above 95%, they come with high investment and operational costs. In recent years, membrane technology has gained attention as a cost-effective alternative.

This talk will discuss the use of high-throughput and AI-driven screening as a rational approach to identifying suitable materials for separation and storage applications. A multi-level screening protocol integrating AI with classical simulation techniques has been employed to evaluate metal-organic frameworks as membrane fillers for biogas upgrading, offering a promising pathway toward more efficient and sustainable purification processes.

Biosketch

Elena Besley is Professor of Theoretical and Computational Chemistry at the University of Nottingham, UK, and a Royal Society Yusuf Hamied Fellow to India (2025). She previously held a Royal Society Wolfson Fellowship (2020–24), supporting outstanding senior scientists. She joined the University of Nottingham as a Lecturer (2011), was promoted to Associate Professor (2014), and became a Professor (2015). Her theoretical and computational work has had a broad impact across multiple disciplines in chemical sciences. For her contributions to theories in charged interactions, she received the Lifetime Achievement Award from the Electrostatics Society of America (2024). Recognitions include Outstanding Female Scientist by Academia Net (2014) and an ERC Consolidator Grant (2013–18). Prof. Besley is also an Associate Editor of Nano Letters.

Integration of CCU in a Coal-to-Methanol Pilot Plant: Bridging the Gap to Net Zero

Prof. Divesh Bhatia

Department of Chemical Engineering,
Indian Institute of Technology Delhi, India

Abstract

The competing demands of energy production and reduced carbon emissions necessitate the development of effective CO_2 management technologies, tailored to the realities of coal- and fossil fuel-driven power and manufacturing sectors in many nations. This talk presents an ongoing consortium project between the Indian Institute of Technology Delhi and Thermax Limited to establish a CO_2 to methanol pilot plant, supported by the Department of Science and Technology, Government of India. The project aims to demonstrate CO_2 capture and its conversion to methanol using both oxygen-deficient syngas and oxygen-rich post-combustion flue gas. By showcasing the CCU technology platform across different industrial sectors, this initiative highlights scalable solutions for CO_2 utilization. The project represents a critical step toward achieving “net zero” by integrating carbon capture with value-added chemical production, setting a precedent for sustainable industrial practices in India and beyond.

Biosketch

Dr. Divesh Bhatia is a Professor in the Department of Chemical Engineering at the Indian Institute of Technology Delhi. He earned his Ph.D. from the University of Houston, Texas. Before joining IIT Delhi in 2014, he worked at Mercedes Benz Research and Development and Nalco Water India Ltd. He leads the Energy and Environment Lab at IIT Delhi, focusing on CO_2 capture and conversion, automotive catalysis, catalytic reduction of greenhouse gases, and gas cleanup technologies. His research contributions have been recognized with several prestigious awards, including the Young Engineers Award from the Institution of Engineers (India) and the Inventor Medal from Daimler AG.

Open Framework Material Catalysts for CO_2 Utilization

Prof. Dinesh Shetty

Department of Chemistry, Khalifa University, Abu Dhabi, UAE

Abstract

CO_2 is a non-toxic, inexpensive, abundant, and renewable carbon source. Developing efficient processes that convert CO_2 into high-value-added products has thus been considered a viable and economical option. Among these processes, photo-/electro-catalytic CO_2 reduction into valuable chemicals has been noted as particularly promising. Open framework materials have emerged as a potential alternative to address many of the issues faced by the current catalysts due to many unique properties: (i) structural tunability and large surface area with numerous spatially isolated docking sites for CO_2 binding, (ii) the inherent pores in the structures facilitate CO_2 adsorption/diffusion through non-covalent interactions, and (iii) conjugated π-electron structure allows for rapid and efficient charge-carrier transport. Considering these merits, we have been working on designing these materials for CO_2 utilization applications. Some of the developed materials showed excellent conversion efficiency without noble metal co-catalysts, a significant positive step in taking these materials for practical applications.

Biosketch

Dr. Dinesh Shetty earned his Ph.D. in Chemistry from Seoul National University, Korea. He conducted postdoctoral research at Emory University, USA; POSTECH, Korea; and NYUAD, UAE, before embarking on his independent career at Khalifa University, UAE, in 2019, where he currently serves as an Associate Professor of Chemistry. Recently, he was awarded the US National Academy of Science Arab American Frontiers Award. He has authored 80 research articles (h-index=33; as of Dec. 2024), over 45 conference papers, delivered more than 35 invited talks, and holds 6 patents. He is an editorial team member for the Chemical Engineering Journal (Elsevier) and RSC Applied Polymers. His research focuses on developing multifunctional polymers and frameworks for applications in energy, water purification/desalination, and resource recovery.

Advanced Materials Characterization for Carbon Capture and Beyond: Use of AI and ML tools

Dr. Rachit Khare

Department of Chemistry and Catalysis Research Center, Technical University of Munich, Germany

Abstract

Advanced and high-throughput materials characterization is crucial for developing efficient carbon capture and utilization (CCU) technologies and furthering their impact beyond just CO_2 mitigation. Achieving sustainability and a circular carbon economy requires a deep understanding of structure-property-performance relationships in catalysts and sorbents, which in turn requires kinetic/mechanistic studies, advanced characterization, and operando techniques assisted by theoretical simulations. However, the complexity and high volume of the generated data necessitates the integration of artificial intelligence (AI) and machine-learning (ML) tools to automate data analysis/processing and accelerate the discovery of new materials. The use of AI/ML techniques dramatically reduces the experimental time and resources. The integration of such tools into catalysis/materials research requires a robust research data management (RDM) strategy and FAIR (Findable, Accessible, Interoperable, Reusable) data practices. An AI/ML-assisted catalysis research and materials characterization workflow will accelerate CCB research while revolutionizing sustainable catalysis, energy storage, and carbon neutrality solutions.

Biosketch

Dr. Rachit Khare is a Group Leader at the Chair II of Technical Chemistry (headed by Prof. Johannes Lercher) at TU Munich (Germany). He earned his B.Tech. in Chemical Engineering from IIT Roorkee (2011) and Ph.D. from the University of Minnesota (USA, 2016) under Prof. Aditya Bhan, focusing on methanol-to-hydrocarbons chemistry on zeolites. After joining TU Munich, he developed operando X-ray absorption spectroscopy setups for heterogeneous catalytic systems. Since 2021, he leads projects on transition metal sulfide catalysts for hydrotreating applications, electrochemical biomass conversion, photochemical H_2 production, and CO_2 conversion to $C2^+$ fuels and chemicals. His research integrates kinetic/mechanistic studies, operando spectroscopy, and molecular simulations with AI/ML tools for deeper insights into heterogeneous catalytic systems.

From Molecules to Processes: Ad Hoc Design of Materials for CO_2 Capture and Utilization by Multiscale Modeling

Prof. Lourdes F. Vega

Research & Innovation Center on CO_2 and Hydrogen, Department of Chemical & Petroleum Engineering, Khalifa University, Abu Dhabi, UAE

Abstract

Aqueous Monoethanolamine (MEA) is the most mature technology for CO_2 capture currently used in industrial processes, the high-regeneration energy consumption being the major obstacle to its large-scale utilization. Different strategies are under investigation to overcome this challenge: (1) the identification of suitable amines as MEA replacements with less energy intensive requirement, (2) the replacement of water (fully or partially) with alternative physical solvents with lower heat capacity and evaporation enthalpy that, when combined with MEA, form physical-chemical absorbents and (3) the use of adsorption into solid materials highly attractive to CO_2 or conveniently modified with amine groups for this purpose. The three alternatives will be explored in this presentation, showing how molecular modeling techniques, combined with machine learning, can help to accelerate the discovery of new materials and solvents. It will also be shown how this molecular information can be used as input data for the process modeling and their techno-economic assessment.

Biosketch

Dr. Vega is a Full Professor in Chemical Engineering and the Director and Founder of the Research and Innovation Center on CO_2 and Hydrogen (RICH) at Khalifa University, UAE. She is a Fellow of the American Institute of Chemical Engineers, an Academician of the MBRAS in the UAE, and the Spanish Royal Society of Science. She has worked across academia and industry in the USA, Spain, and the UAE. With over 300 publications and six patents under exploitation, she is recognized for translating fundamental science into applications in clean energy and sustainable products, focusing on CO_2 capture and utilization, hydrogen, sustainable fuels, and cooling. She has led major industrial-academic consortia, including SOST-CO_2 (focused on CCB) with 14 companies and 30 academic institutions. A leading expert in CCB, she has received several prestigious international awards.

Application of AI in Carbon Capture and Beyond

Prof. Hariprasad Kodamana

Indian Institute of Technology Delhi - Abu Dhabi, UAE

Abstract

Artificial Intelligence (AI) is revolutionizing carbon capture and utilization (CCU) by enabling rapid knowledge extraction, material discovery, and process optimization. There have been various attempts in the research community to develop novel pathways that mitigate and control this impact. Our research leverages AI-driven models to accelerate CCU technologies and extends its impact to broader sustainable energy applications. These outcomes of their research are primarily documented in articles, and finding effective solutions necessitates the ability to scan the scientific literature and extract relevant information. In this talk we speak about, CCU-Llama, a domain-specific large language model (LLM), based on Llama-2, that mines scientific literature to extract insights on adsorption materials, catalysts, and reaction pathways for CO_2 capture and conversion. Complementing this, machine learning-based photocatalyst screening integrates text mining hydrogen production. These methodologies enhance material performance prediction, energy efficiency, and life cycle assessments, fostering AI-powered solutions for a carbon-neutral and sustainable future.

Biosketch

Hariprasad Kodamana is an Associate Professor IIT Delhi - Abu Dhabi (on secondment) and IIT Delhi with a joint appointment in the Department of Chemical Engineering and the Yardi School of Artificial Intelligence. Prof. Kodamana's research interests encompass various interdisciplinary fields, including artificial intelligence and machine learning, optimization and control, and sustainable and net-zero systems within the broader scope of process systems engineering. With over a decade of experience, he has developed innovative algorithms that integrate computational models and machine learning to drive the efficiency and sustainability of complex chemical and energy systems. He is serving as a subject editor for two international journals in his areas of expertise.

Generative AI for Sustainability

Dr. Alex Aliper

Insilico Medicine, Abu Dhabi, UAE

Abstract

Recent advances in generative AI and robotics have set new speed and cost benchmarks in drug discovery, significantly outperforming traditional methods. These innovations extend beyond healthcare. New generative chemistry methods enable the development of novel materials for effective CO_2 capture, hydrogen storage, sustainable agriculture and other industrial applications that may significantly impact environmental sustainability. This talk will provide an overview of these advances in AI for good and discuss the future implications on sustainability.

Biosketch

Alex Aliper, PhD, is the President of Insilico Medicine. He pioneered the application of AI in multi-omics data for drug discovery and drug repurposing, generative chemistry and generative biology and put an AI-designed drug into human clinical trials. Alex Aliper built a team of over 100 AI engineers that developed state-of-the-art software products for target discovery, small molecule generation and clinical trial outcome prediction. He was recognised as "Top 100 AI Leaders in Drug Discovery and Advanced Healthcare" by Deep Knowledge Analytics. In 2020 Endpoint News selected Alex Aliper as the top 20 under 40 biotechnology executives globally.

Advances in Reactor Design for Carbon Capture and Beyond

Prof. Sreedevi Upadhyayula

Department of Chemical Engineering,
Indian Institute of Technology Delhi, India

Abstract

Carbon Capture and Conversion processes typically begin at the molecular scale, followed by the reactor scale for design and operation, and finally, the process scale for integration and intensification. Molecular-scale studies involve theoretical density functional theory calculations to determine the interaction energy bounds between reactant molecules, catalysts, and other molecules in the reaction phases. This approach aids in developing the optimal catalytic composition, which is then tested through laboratory-scale reactor investigations to identify the best operating conditions and suitable reactor types. The reaction mechanism and kinetics, then, help to develop a feasible model that can be used in the reactor design. The reactor type and process scale are highly related to the process efficiency and CO_2 capture and conversion costs. Advanced design considerations start from feed distributor design to CO_2 concentration in the feed mixture while sizing the reactor and finding trade-offs between higher feed reactant ratios to energy requirements management.

Biosketch

Prof. Sreedevi Upadhyayula is CLASS of 66 Chair Professor in the Department of Chemical Engineering at IIT Delhi. After earning her M.Tech in Chemical Engineering from IIT Kharagpur in 1993, she worked as a Senior Design Engineer in both public (BHPV Ltd.) and private sectors (APL, Chennai). She returned to academics in 1998, completing her Ph.D. in 2001 from NCL, Pune, and IIT Kharagpur. She pursued post-doctoral research at the University of Notre Dame, USA, before joining IIT Kharagpur in 2004 and IIT Delhi in 2006. Her research focuses on environmentally benign heterogeneous catalysis, ionic liquids, zeotype materials, and biomass conversion to biofuels, emphasizing catalyst design, kinetics, and modeling for petrochemical and refinery processes.

Tuning the Physicochemical Attributes of Catalytically Active Materials for Better Understanding of Struture-Property-Performance Triad

Prof. Manjesh Kumar

Department of Chemical Engineering,
Indian Institute of Technology Delhi, India

Abstract

Climate change is an existential threat that requires immediate attention to explore sustainable solutions such as the integration of renewable energy and implementation of carbon capture, utilization, and storage (CCUS) technologies. To this end, we are exploring two classes of material; 1) Titania, and 2) Nanoporous zeolites with direct relevance to energy transformation and CCUS. We delve deeper to understand the mechanistic principles of growth phenomenon to tune the physicochemical attributes of microscopic crystals. We will showcase the complex blueprint of the crystallization phenomenon resulting in particles of different shapes, sizes, porosity, and elemental composition. Overall, the tuning of properties including, size, morphology, crystal planes, Al speciation, porosity speciation, and Ti-site speciation have direct implications on the performance of these materials. Here, we will showcase innovative green pathways for developing a single-pot method for generating core-shell zeolite which can be used as an efficient adsorbent. Overall, we will present comprehensive design principles for tuning the advanced functional materials amenable to desired performance.

Biosketch

Prof. Manjesh Kumar's research group is focused on developing 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 a wide variety of targeted applications in catalysis and gas separation such as reverse water gas shift reaction, hydrocarbon cracking, CO_2 electrochemical reduction, methanol to olefins, alkylation, CO_2 capture, and H_2 separation among others. To obtain the efficient material, we delve deeper into the fundamental studies to develop the growth mechanism which in turn helps generate heuristics for crystal design.

Capture and Electrochemical Conversion of Carbon Dioxide

Prof. Ahsanulhaq Qurashi

Department of Chemistry, Khalifa University, Abu Dhabi, UAE

Abstract

The escalating levels of atmospheric carbon dioxide (CO_2) exceeding 425 ppm, driven by the extensive use of fossil fuels and other greenhouse gas emissions, necessitate a shift toward clean energy production to mitigate climate change. While carbon capture, storage, and utilization have been key strategies for carbon management, relatively less attention has been given to the direct conversion of CO_2 into clean fuels and value-added chemicals as a sustainable feedstock. Direct CO_2 capture presents a renewable pathway for producing carbon monoxide (CO), which can subsequently be upgraded into high-value products. This presentation will explore emerging trends in direct capture and electrochemical CO_2 conversion, highlighting recent advancements in catalyst development for electrochemical CO_2 splitting. Additionally, the challenges, frontiers, and opportunities associated with durable materials for CO_2 conversion will be discussed, providing insights into future directions for sustainable carbon utilization.

Biosketch

Dr. Ahsanulhaq Qurashi is a materials chemist and nanotechnologist, an Associate Professor at Khalifa University, Abu Dhabi. He is also a visiting faculty member at EPFL Switzerland, Tokyo University, Nagoya University, and CALTECH. He has published over 140 peer-reviewed articles and presented more than 80 papers at international conferences. His research focuses on new materials and hybrids, exploring structure-property relationships for energy conversion, including green hydrogen production, CO_2 conversion, and energy storage. He holds six USPTO patents. Dr. Ahsan serves on the editorial boards of Materials Research Bulletin, Energy and Environmental Materials, and Ultrasonics Sonochemistry and is an external editor for Nature Communications Engineering. A Fellow of the Royal Society of Chemistry (FRSC), he is also a member of the Mohammed Bin Rashid Academy of Scientists (MBRAS).

Strategic Approaches for CO_2 Emissions Reduction in Steel, Power and Transportation Industries

Prof. Ejaz Ahmad

Department of Chemical Engineering,
Indian Institute of Technology (Indian School of Mines), Dhanbad, India

Abstract

Carbon capture, sequestration, and utilization are the most discussed topics worldwide due to CO_2 determinantal effects on the environment. Indeed, a wide range of technologies have been developed to tackle emitted CO_2, yet few research areas, that have very high potential to reduce greenhouse gas emissions, have been overlooked for decades. The reduction of CO_2 emission at the source via a carbon-neutral approach has not been explored in detail. For example, the use of waste biomass-derived bio-coal has the potential to reduce steel industry CO_2 emissions by up to 40%. Similarly, blending agro residues in thermal power plants can reduce overall CO_2 emissions. Moreover, the use of biorenewable fuels and additives has the potential to reduce CO_2 emissions in the transportation sector. Thus, the present study discusses different strategic and innovative approaches to reduce CO_2 emission at the source by partial replacement of fossil fuels with biorenewable energy sources.

Biosketch

Dr. Ejaz Ahmad is an esteemed Assistant Professor in the Department of Chemical Engineering at IIT (ISM) Dhanbad, where he also serves as the Head of the Naresh Vashisht Centre for Hydrogen and CCUS Technologies and Faculty In-Charge of Sponsored Research & Industrial Consultancy. A trailblazer in heterogeneous catalysis, his research drives innovations in bio-renewable energy, sustainable aviation fuel, turquoise hydrogen, green gasoline, waste-to-wealth, and urban mining. His pioneering biomass-to-biofuel and bio-coal technology holds the potential to reduce GHG emissions in the steel industry by 18-40%, marking a significant step toward industrial decarbonization. A two-time recipient of India's prestigious Gandhian Young Technological Innovation (GYTI) Award, he has been honoured by both the President of India and the Science and Technology Minister.

The Art of Designing Multifunctional Catalysts for Value-Added Products: Fundamentals and Beyond

Prof. Kyriaki Polychronopoulou

Mechanical & Nuclear Engineering and Center for Catalysis and Separations (CeCaS), Khalifa University, Abu Dhabi, UAE

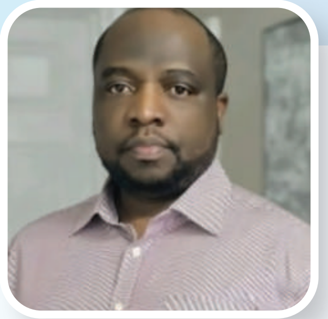
Abstract

Catalysis lies at the core of many fuel-related deployment technologies, particularly in the transformation of waste into energy and fuels. This sector is projected to reach a revenue of USD 54.8 billion by 2027, with a compound annual growth rate (CAGR) of 7.4% from 2020 to 2027. In alignment with the UAE Energy Vision 2050, carbon capture, utilization, and storage (CCUS) research is of strategic priority for the United Arab Emirates. The catalytic conversion of CO_2 into valuable chemicals and fuels offers a promising approach for mitigating carbon emissions and advancing carbon neutrality. Catalytic materials can be tailored for use as conventional, photocatalytic, or photoelectrocatalytic systems, enabling the efficient conversion of CO_2 into products such as formic acid, methanol, methane, and others. Key challenges remain in overcoming the thermodynamic and kinetic barriers associated with CO_2 activation, which are critical to advancing these technologies.

Biosketch

Kyriaki Polychronopoulou is a Full Professor of Mechanical and Nuclear Engineering since 2020 and served as Acting Chair in 2024. She is the Founding Director of the Center of Catalysis and Separations (CeCaS) at Khalifa University and a Visiting Professor at ETH-Zurich. CeCaS, a strategic center at Khalifa University, supports UAE's energy transition and alternative fuels.Prof. Polychronopoulou is also the Founder, CEO, and CTO of two CeCaS spin-offs. She has been listed in Stanford University's Top 2% Scientists (2020–2023) and ranks in the top 0.5% on Scholar GPS. Since May 2021, she has been an elected regular member of the Mohammed Bin Rashid Academy of Scientists (MBRAS).

New Industrial Approaches for Carbon Capture and Beyond



Dr. Mathew Aneke

Wood, UAE

Abstract

Carbon capture, utilization, and storage (CCUS) is widely recognized as a critical component of global decarbonization efforts, particularly for hard-to-abate sectors. Early CCS projects followed a point-to-point model, where a single large emitter, such as a fossil-fuel power plant, was connected to a nearby CO_2 storage site. While this approach remains commercially viable for large-scale emitters, it is not economically feasible for smaller sources due to the high costs associated with dedicated CCUS infrastructure. To enhance economic viability and accommodate emitters of varying scales, the industry has shifted toward hub-and-cluster models, where multiple emitters share CO_2 transport and storage infrastructure. Although this approach improves cost efficiency, it introduces complexities in designing and operating CCUS networks, particularly due to variations in CO_2 stream composition from different sources. This study examines the challenges associated with establishing CO_2 specifications for transport pipelines within industrial clusters, addressing key considerations for ensuring safe and efficient infrastructure deployment.

Biosketch

Dr. Aneke is a seasoned professional with over 20 years of experience in academia, research, and industry. His expertise spans CCUS, Waste to Energy (pyrolysis, thermal and plasma gasification), Low Carbon Technologies, Biorefinery, Energy Storage, Hydrogen technologies, Bioenergy, Energy Efficiency, Combined Heat and Power, Trigeneration Systems, HVAC, Waste Heat Recovery, and Energy Transition.He holds a bachelor's in Chemical Engineering from Federal University of Technology Owerri, Nigeria, a master's in Process Systems Engineering from Cranfield University, UK, and a PhD in Process and Energy Systems Engineering, UK. He is a Fellow of the UK Higher Education Academy, a Chartered Engineer with the UK Engineering Council, and Chairman of the Industry Advisory Board at Newcastle University. He is a member of several international engineering bodies, including Energy Institute, HEXAC, PRO-TEM, IChemE, and Institute of Gas Engineers and Managers.

Three stage CCUS integration in industrial landscape: End of Pipe (EOP), CO_2 Compliant Designs (CCD), CCUS in One Pot (COP)

Prof. R. R. Sonde

Indian Institute of Technology Roorkee, India

Abstract

CCUS is vital for achieving global net-zero emissions, but its integration into industrial infrastructure is influenced by sector-specific factors, technology maturity, and plant lifespan. This talk discusses the three stages of CCUS implementation, starting with End-of-Pipe (EOP) solutions, where TRL 7 technologies are scaled to TRL 9 through innovations in process design, new solvents, energy integration, and life-cycle management, currently applied in industries such as cement, steel, and power. The next stage focuses on designing new plants with built-in CCUS compatibility to overcome the limitations of EOP solutions, with ongoing work advancing towards pilot-scale implementation. Finally, the most transformative stage involves the direct conversion of CO_2 into fuels, chemicals, and commodities within integrated processes, requiring significant funding and industry collaboration to achieve breakthroughs. This presentation will explore the R&D needs at each stage to accelerate the widespread adoption of CCUS technologies.

Biosketch

Dr. Sonde began his career as a scientist at BARC, where he topped his batch in nuclear science and engineering, earning the Dr. Homi Bhabha Gold Medal. He played a key role in India's nuclear energy program, specializing in isotope separation and heavy water production, making India a global leader in this technology. After 23 years, he joined NTPC as Executive Director, establishing "Energy Technologies" (now NETRA) to advance clean coal, IGCC, carbon capture, and hybridization. He pioneered India's CCUS strategy and led major projects, including coal-to-methanol and hydrogen-powered vehicles. Consulting for ADB, he explores CO_2 storage in abandoned wells. Recognized with prestigious awards, he mentors students and delivers global talks on deep-tech solutions.

Opportunities for Innovations in CCB: Developing a Multi-Level Perspective

Prof. M. Ali Haider

Indian Institute of Technology Delhi - Abu Dhabi, UAE

Abstract

Scientific innovation thrives on continuous experimentation and learning, but not all lab discoveries transition smoothly into industry due to entrenched technological regimes shaped by science, culture, policy, and investment. Disrupting these systems requires a top-down approach. To achieve net-zero emissions, we propose a multi-level strategy incorporating disruptive technologies like zero-emission coal, third-generation power systems, and CO_2 conversion. Our lab explores innovative catalyst materials for efficient fuel use and CO_2 reduction using quantum mechanical DFT simulations to guide rational design. We advocate an in silico, high-throughput approach to catalyst tailoring, aiming for transformative breakthroughs in Carbon Capture and Beyond (CCB).

Biosketch

Prof. M. Ali Haider is the Vice Provost for Research and External Engagement at the IIT Delhi-Abu Dhabi. He holds an M.S. and Ph.D. in Chemical Engineering from the University of Virginia and a B.Tech. from IIT Guwahati. He is an Editorial Advisory Board member for ACS Sustainable Chemistry & Engineering. In 2023, he visited the Catalysis Research Center at Technical University Munich as an Alexander von Humboldt fellow. He has been recognized by the Royal Society of Chemistry as an 'Emerging Investigator,' 'Highly Cited Author,' and for his work in the 'Editor's Choice Collection.' He was a visiting fellow at the University of Delaware's Catalysis Center for Energy Innovation, supported by the Indo–US Science and Technology Forum. He received the 'Dr. A.P.J Abdul Kalam HPC Award for R&D in HPC Application' from Hewlett Packard Enterprise and Intel. Prof. Haider is a member of NASI and INYAS and actively promotes science on sustainability and climate change.

Decarbonizing Energy Storage and Utilization: Pathways for a Low-Carbon Future

Prof. Dibakar Rakshit

Indian Institute of Technology Delhi - Abu Dhabi, UAE

Abstract

As the world accelerates its transition to a low-carbon economy, Carbon Capture, Utilization, and Storage (CCUS) has emerged as a key enabler of deep decarbonization. However, the efficiency and feasibility of CCUS systems depend significantly on energy management strategies, particularly for high-temperature industrial processes and power generation. This presentation will explore the integration of high-temperature latent heat storage (HT-LHS) with supercritical CO_2 (sCO_2) Brayton cycles as a pathway to enhance energy efficiency in CCUS applications. Thermal energy storage, particularly at high temperatures, plays a crucial role in reducing energy losses and optimizing heat utilization in post-combustion carbon capture and direct air capture systems. Additionally, sCO_2 cycles offer high thermal efficiency and reduced compression work, making them an ideal candidate for minimizing the energy penalty associated with CCUS operations. This presentation will highlight key advancements in latent heat storage system design, experimental validation of numerical models, and techno-economic comparisons with alternative storage solutions. Further discussion will cover waste heat recovery in cement plants and its potential for CO_2 mitigation, along with the role of carbon markets in incentivizing industrial decarbonization. The talk will conclude with insights into hybrid energy storage strategies and the integration of CCUS with hydrogen and renewable energy technologies, ensuring a sustainable and economically viable path toward net-zero emissions.

Biosketch

Prof. Dibakar Rakshit is currently a Professor at IIT Delhi-Abu Dhabi and Department of Energy Science and Engineering at Indian Institute of Technology Delhi (IIT Delhi). He has twenty years of experience in thermofluid sciences pertaining to design and optimization of energy systems. His Ph.D. at The University of Western Australia involved studies of multiphase mass transfer phenomenon related to thermal diffusion of Liquefied Natural Gas (cryogenic fluids). From there, Dr. Rakshit developed his deep interest in thermal energy storage and pursued it further in his post-doctoral research at Australian Solar Thermal Research Initiative (ASTRI), CSIRO, Australia.

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