المعهد الهندي للتكنولوجيا دلهي أبوظبي

INDIAN INSTITUTE OF TECHNOLOGY DELHI ABU DHABI

AiMS2025

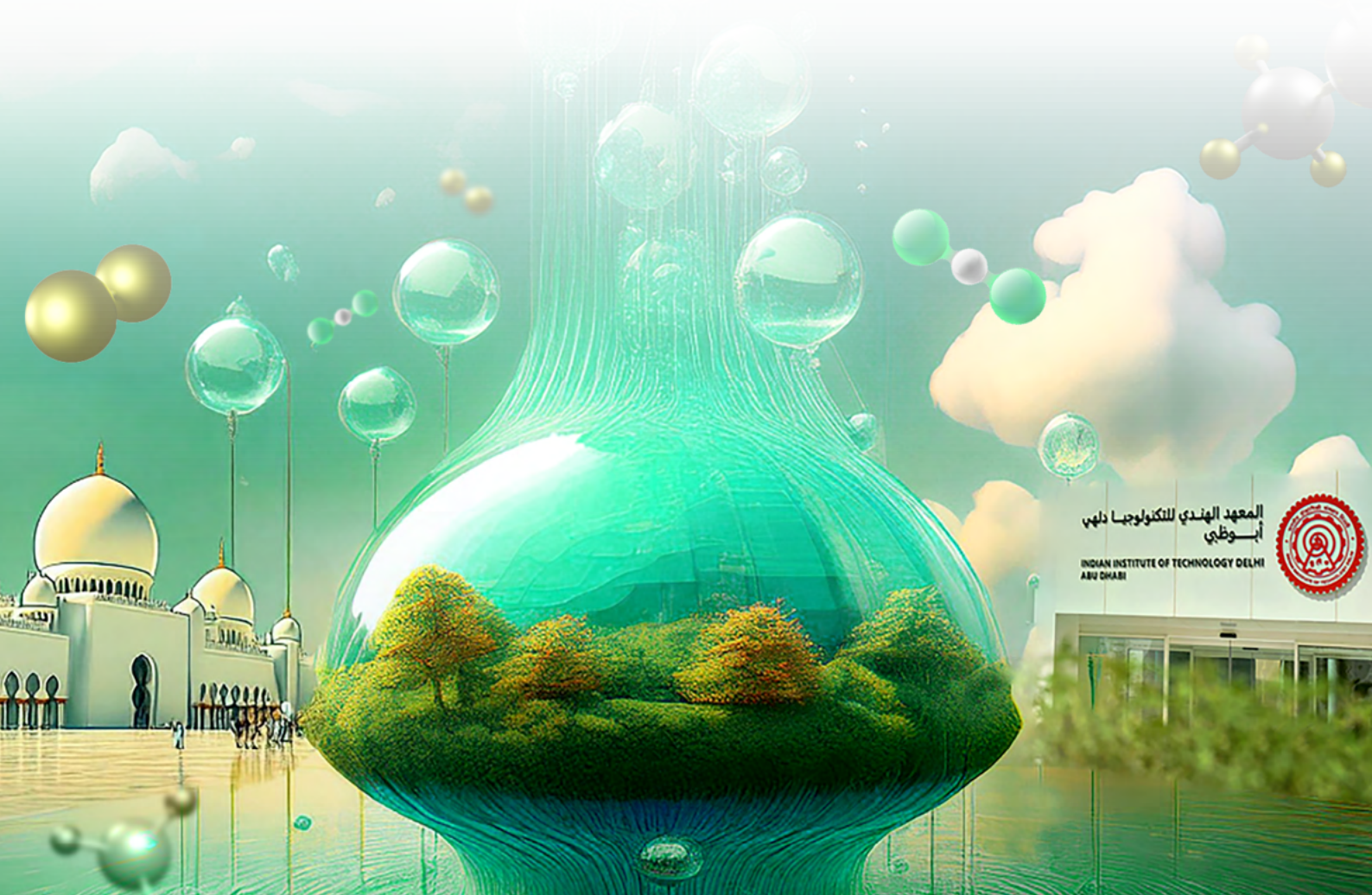
AI & MATERIALS FOR SUSTAINABILITY

International Conference on AI and Materials for Sustainability

Water – Energy – Climate

15th - 17th December, 2025

Organised by **IIT Delhi - Abu Dhabi**



About the Conference

The **International Conference** on **Artificial Intelligence and Materials for Sustainability** (AIMS 2025), hosted by the **Indian Institute of Technology Delhi – Abu Dhabi**, brings together experts from around the world to explore the intersection of AI and materials science in addressing global sustainability challenges.

This three-day conference provides a platform for leading researchers, scientists, and engineers to present peer-reviewed research, share insights, & engage in discussions on the latest advancements in sustainable technologies. As the flagship international conference of IIT Delhi's first overseas campus, **AIMS 2025** highlights cutting-edge research and innovation aimed at creating a more sustainable future for society and the environment.

Conference Objectives

AIMS 2025 is predicated on the scientific consensus that breakthroughs in energy, water, and environmental systems are intrinsically linked to the integration of Artificial Intelligence, which is accelerating the cycle of material discovery, design, and aiding sustainability.

The primary objectives of the conference are:

- **To disseminate original, high-impact research findings** through plenary, keynote lectures, invited talks, peer-reviewed oral and poster presentations.
- **To bridge fundamental scientific discovery** with industrial application by connecting academic researchers with industry practitioners and policymakers.
- **To foster the next generation of scientists** by providing a platform for presentations and networking.

Core Scientific Themes

AIMS 2025 showcases breakthroughs in sustainable materials, hydrogen, carbon capture, and AI-driven energy solutions. Overall themes of the conference listed below highlights the importance of using AI in solving problems related to water, energy and climate future.

1. **Carbon Capture and Beyond (CCB):** Materials, processes, and decarbonization of hard-to-abate sectors, CO_2 capture & CO_2 valorisation.
2. **Innovations in Hydrogen Production and Management:** Innovations in green and blue hydrogen, and materials for hydrogen storage.
3. **Materials for Sustainable Energy:** Energy storage materials and solutions, water purification, water splitting, and methane abatement.
4. **Materials and AI in Circular Energy Transitions:** Advances in AI methods, life cycle assessment, and techno-economic evaluation, AI based approach in circular economy and sustainable materials.
5. **AI for Material Design:** AI in materials discovery and design for a sustainable future, AI-quantum mechanical integration, and high -throughput material screening.
6. **Digital Sustainability:** Data-driven models, research database management, and decarbonising data centers.
7. **The Water-Energy-Climate Nexus:** Predictive modelling, AI-powered accelerated modelling for water, energy and climate futures.
8. **Industry-Academia Collaboration for AIMS:** Bridging the gap for sustainable innovation.
9. **Integrating Science, Engineering, and Policy for AIMS**

Organized by
IIT Delhi - Abu Dhabi

The **Indian Institute of Technology Delhi** (IIT Delhi) is one of India's premier institutions for education and research in science, technology, and engineering. **IIT Delhi - Abu Dhabi**, its international campus, represents a visionary step in extending IIT Delhi's legacy to the dynamic innovation ecosystem of the UAE.

Located in Khalifa City B, Abu Dhabi, this campus is the result of a strategic collaboration between India and the UAE, aimed at advancing excellence in education, research, and innovation. With a focus on cutting-edge fields such as artificial intelligence, sustainable technologies, and advanced computing, **IIT Delhi - Abu Dhabi** is poised to emerge as a global hub for transformative academic and industry-led initiatives.

Pioneering Speakers

Visionary leaders shaping the global sustainability - where science meets innovation & ideas become action.

50+ Distinguished and Invited Speakers

Pre-Conference Workshops

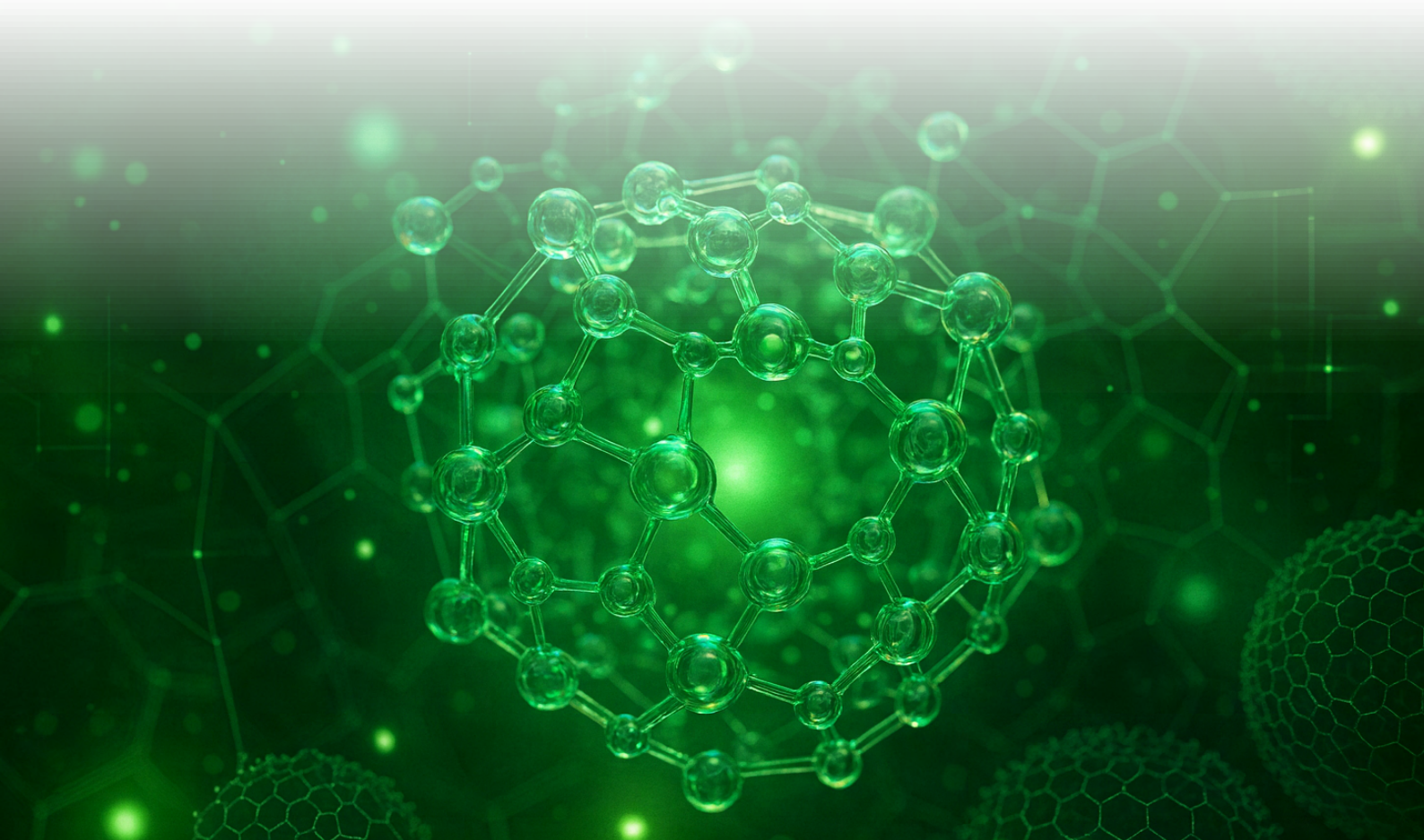
The workshops will provide an interactive platform for participants to engage and offers direct engagement with attendees and will enhance your organization's visibility in the academic and professional community.

Workshop 01: Research Data Management for Catalysis and Materials Research (NFDI4Cat and SPARC)

Workshop 02: Why High-Quality Presentations and Posters Matter? (American Chemical Society)

Workshop 03: Innovation and Lab-to-Industry Pathways (American Chemical Society)

Workshop 04: Hands-on with Data-Driven Approaches to Accelerate Catalysis and Materials Research (Meta)



Journal Special Issues

In collaboration with leading journals, the AIMS 2025 conference will provide unparallel visibility and recognition in the scientific community.

Computers & Chemical Engineering

Publisher: Elsevier

Special Issue Title: International Conference on AI and Materials for Sustainability (AIMS-2025)

Focus: Integration of AI tools in chemical engineering and materials sustainability

ACS Sustainable Chemistry & Engineering

Publisher: American Chemical Society (ACS)

Virtual Special Issue: Artificial Intelligence Tools - A New Frontier for Sustainability

Focus: Innovative AI-driven approaches for sustainable chemistry and engineering

ACS Sustainable Resource Management

Publisher: American Chemical Society (ACS)

Virtual Special Issue: Artificial Intelligence Tools - A New Frontier for Sustainability

Focus: Advances in AI applications for resource optimization, recycling, and circular economy

Awards and Recognition

AIMS 2025 celebrates excellence in research and innovation by recognizing outstanding contributions from participants across oral and poster presentations. These awards will highlight the creativity, impact, and quality of work presented during the conference.

Best Oral Presentation Awards: Recognizes presenters who deliver original, high-impact research with clarity and engagement. Multiple awards are given across different themes.

Poster Presentation Awards: Honors exceptional poster presentations that demonstrate innovation and scientific rigor.

Oral and Poster Awards by: ACS Sustainable Chemistry & Engineering, Industrial & Engineering Chemistry Research, Energy & Fuels, ACS Applied Energy Materials, ACS Omega, ACS Engineering Au, ACS Sustainable Resource Management, ACS Physical Chemistry Au, ACS Materials Au and ACS Environmental Au.

Distinguished and Invited Speakers Biosketch

Johannes A. Lercher

Technical University of Munich, Germany

Johannes Lercher is Professor emeritus of Chemistry at the TU München and was Director of the Institute of Integrated Catalysis at the Pacific Northwest National Laboratory. His current research addresses fundamental aspects of catalysis lowering the carbon footprint via radically new approaches. Being member of several academies, he served as long-time Editor-in-Chief of the Journal of Catalysis, President of the International Zeolite Association and the European Federation of Catalysis Societies. His contributions to research have been recognized by awards such as the Michel Boudart Award of the North American Catalysis Society and the European Federation of Catalysis Societies, the Alwin Mittasch Prize of DECHEMA, and the ENI Award for Hydrocarbon Research.

Ahmed Al Hajaj

Khalifa University, UAE

Ahmed Al Hajaj is a faculty member at the Department of Chemical and Petroleum Engineering at Khalifa University and the CCS theme lead at the Research and Innovation Center for CO_2 and Hydrogen (RICH). He is currently a Visiting Fellow at the University of New South Wales and previously served as a Visiting Professor at MIT. He holds a B.Sc. in Mechanical Engg. from the University of Arizona, an M.Sc. from the University of Miami and Imperial College London, and a Ph.D. in Chemical Engg. from Imperial College London. His research spans process systems engineering, optimization, product synthesis, and process control. He integrates multiscale modeling, CFD simulations, and experimental studies to develop systematic tools for low-carbon and sustainable industrial technologies.

Fengqi You

Cornell University, USA

Fengqi You is the Roxanne E. and Michael J. Zak Professor in Energy Systems Engineering at Cornell University, with affiliations across nine graduate fields, including Chemical Engineering, Computer Science, Electrical and Computer Engineering, among others. He serves as Co-Director of the Cornell University AI for Science Institute (CUAISci), Co-Director of the Cornell Institute for Digital Agriculture (CIDA), and Director of the Cornell AI for Sustainability Initiative (CAISI). Before joining Cornell, he worked at Argonne National Laboratory and served on the faculty at Northwestern University. He is the recipient of several prestigious awards including the NSF Career Award, Amazon Research Award, and the Lawrence K. Cecil Award in Environmental Chemical Engineering.

Shobhana Narasimhan

JNCASR, India

Shobhana Narasimhan is a Professor of Theoretical Sciences at the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bengaluru, where she leads the Computational Nanoscience Group. Her research uses density functional theory to understand and design nanomaterials with tailored properties. She earned her Ph.D. from Harvard University and completed postdoctoral work at Brookhaven National Laboratory and the Fritz Haber Institute in Berlin. She is an International Honorary Member of the American Academy of Arts and Sciences and a Fellow of the APS, the Indian Academy of Sciences, and the National Academy of Sciences, India. She also actively works to promote gender and regional diversity in science.

Maryam Al Nahyan

New York University Abu Dhabi, UAE

Maryam Al Nahyan is a Faculty of Mechanical Engineering at the New York University Abu Dhabi. Al Nahyan received her Bachelor's degree in Chemistry from the UAE University (2016), Master's Degree in Chemical Engineering from Masdar Institute in Collaboration with MIT (2018), and Ph.D. in Materials Science and Engineering from Khalifa University (2024). Al Nahyan's research interests span the fields of advanced energy storage and material synthesis. Nahyan's passion for science and technology is matched only by her sense of duty to the UAE society and the UAE leadership's vision. Being a passionate educator and dedicated researcher, she is committed to advancing the field of scientific research in the UAE.

Jeffrey Snyder

Northwestern University, USA

Jeffrey Snyder is a Professor of Materials Science and Engineering at Northwestern University, where he leads research on thermoelectric and energy-related functional materials. His research focuses on developing new permanent magnets, analyzing electrical and thermal interface resistance in semiconductors, and engineering grain boundaries and band structures for high thermoelectric performance. He earned his Ph.D. and MS in Applied Physics from Stanford University and a BA from Cornell University. His work spans solid-state physics, thermodynamics of thermoelectric materials, Zintl phases for power generation, and advanced high-temperature transport measurements, contributing to innovations in energy-efficient materials and thermoelectric engineering.

Bhavik Bakshi

Arizona State University, USA

Bhavik Bakshi is the Wrigley Professor at Arizona State University, with appointments in the School for Engineering of Matter, Transport and Energy, the School of Sustainability, and the School of Complex Adaptive Systems. His research develops systematic methods to enable engineering solutions that drive sustainable transformation while respecting ecological limits. He focuses on product, process, supply-chain, and landscape design for a sustainable circular economy. His contributions include a widely used textbook on sustainable engineering, user-friendly software tools, and international short courses. He has received numerous honors, including major AIChE awards, NSF CAREER award, and recognition from the American Council for LCA.

Joseph Smith

Missouri University of Science and Tech., USA

Joseph D. Smith was the inaugural Wayne and Gayle Laufer Endowed Energy Chair (2011 – 2021) at Missouri S&T. He also served as director of the Energy Research & Development Center (2013–18) and as Executive Director of the Small Modular Nuclear Reactor R&D Consortium (2013–16). He has over 30 years of experience in the chemical and petrochemical industries, with roles at Dow (1990–97), Cabot, Koch Industries, and Idaho National Laboratory, specializing in combustion, gasification, reactive-flow CFD modeling, process heaters, and gas-flare performance. Dr. Smith has founded several engg. startups and has previously held faculty positions at Tennessee Technological University, the University of Michigan, the University of Illinois at Urbana-Champaign, & the University of Tulsa.

Ramakrishna R. Sonde

BITS Pilani, Goa Campus, India

R.R. Sonde is Professor Emeritus at BITS, have been associated with six IITs, Chair of ESTIC's Energy, Environment & Climate (EEC) vertical for "Developed India @2047," and a Board Member of AcSIR under CSIR. After his career as a scientist at BARC, he became Executive Director at NTPC, where he founded the Energy Technologies group (now NETRA) and pioneered India's early work on IGCC, clean-coal technologies, and CCUS. His recent leadership includes high-ash coal-to-methanol, hydrogen-based systems, sodium–sulfur batteries, and the DST-funded Hydrogen Valley program at IIT Jodhpur. He continues to advance CCUS pilot facilities, advise the ADB on CO_2 storage, and guide national decarbonization strategies across various industries.

Jorge Gascon

KAUST, Saudi Arabia

Jorge Gascon is a Professor of Chemical and Biological Engineering at King Abdullah University of Science and Technology, where he leads the Advanced Catalytic Materials group. His research focuses on developing catalysts and porous materials, including MOFs, zeolites, and multifunctional hybrid systems for energy conversion, CO_2 utilization, and sustainable chemical processes. He earned his PhD in Chemical Engineering from the University of Zaragoza and conducted postdoctoral research at TU Delft, where he later became a faculty member before joining KAUST. Prof. Gascon has published extensively in the fields of catalysis, materials design, and reaction engineering, and his work bridges fundamental materials chemistry with industrially relevant processes.

Marc-Olivier Coppens

University College London, United Kingdom

Marc-Olivier Coppens is Ramsay Memorial Professor in Chemical Engineering at University College London and directs the Centre for Nature-Inspired Engineering, founded through an EPSRC “Frontier Engineering” Award. He has pioneered nature-inspired chemical engineering (NICE) for 25 years, developing systematic methodologies to accelerate sustainable innovation in energy, chemical manufacturing, water, and health. He is a Fellow of IChemE, AIChE, and RSC; Corresponding Member of the Saxon Academy of Sciences (Germany); Qiushi Professor at Zhejiang University (China); Scientific Council Member for IFP Energies nouvelles (France); has published over 200 journal articles; and is Editor-in-Chief of Chemical Engineering and Processing: Process Intensification.

Hassan Arafat

Khalifa University, UAE

Hassan Arafat is the Senior Director of the Research and Innovation Center for Graphene & 2D Materials (RIC2D) and a Professor of Chemical Engineering at Khalifa University. He previously directed KU’s Center for Membranes and Advanced Water Technology (CMAT) and has held positions at Argonne National Laboratory, An-Najah University, Utah State University, and MIT. He received his Ph.D. in Chemical Engineering from the University of Cincinnati. His work focuses on graphene and 2D materials, membrane desalination, and the development of sustainable desalination systems. He serves on the selection committees of the Zayed Sustainability Prize & the Mohammed bin Rashid Al Maktoum Global Water Award and has received major national & international honors.

Zachary W. Ulissi

Meta Fundamental AI Research, USA

Zachary W. Ulissi is a Senior Research Manager at Meta's Fundamental Artificial Intelligence Research (FAIR) organization, where he co-leads the FAIR Chemistry team developing AI and ML methods for materials, chemistry, climate technologies, and Meta's augmented-reality and virtual-reality hardware programs. He is also an Adjunct Professor of Chemical Engineering at Carnegie Mellon University. He previously served as an Assistant and Associate Professor at Carnegie Mellon University before joining Meta in 2023. He completed his Ph.D. in Chemical Engineering at MIT and postdoctoral research at Stanford University. His work integrates machine learning with quantum chemistry and molecular simulations to design novel catalysts and materials.

David Flaherty

Georgia Institute of Technology, USA

David W. Flaherty is a Professor of Chemical and Biomolecular Engineering at the Georgia Institute of Technology and the Thomas C. DeLoach Jr. Endowed Professor. He earned his Ph.D. at the University of Texas at Austin and conducted postdoctoral research at UC Berkeley. His research combines kinetics, spectroscopy, and materials design to elucidate reaction mechanisms at solid–liquid and solid–gas interfaces, advancing understanding of solvent and confinement effects and unifying concepts across thermo- and electrocatalysis. He is Editor-in-Chief of the Journal of Catalysis and a recipient of major awards, including the DOE Early Career Award, NSF CAREER Award, and the 2026 Paul H. Emmett Award in Fundamental Catalysis.

Xiaonan Wang

Tsinghua University, China

Xiaonan Wang is a faculty member in the Department of Chemical Engineering at Tsinghua University. She received her B.Eng. from Tsinghua University and her Ph.D. from the University of California, Davis, followed by postdoctoral research at Imperial College London. She previously served as an Assistant Professor at NUS, where she led the Smart Systems Engineering group and is Deputy Director of Singapore's Accelerated Materials Development Programme. Her research develops intelligent computational methods: multiscale modeling, optimization, data analytics, and machine learning for materials, energy, environmental, and manufacturing systems. She serves on the editorial boards of major journals and has received multiple international young researcher and best-paper awards.

Marco Saitta

Université Pierre et Marie Curie - France

A. Marco Saitta is a Physics Professor at Sorbonne Université, currently transitioning from the Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie to the Laboratoire de Physique de l'École Normale Supérieure in Paris. His research focuses on the Physics of Transition, combining AI-driven modeling with materials physics to address challenges in energy, water, and sustainability. Originally specialized in first-principles simulations and matter under extreme conditions, he now develops machine-learning interatomic potentials and studies complex, disordered materials relevant to the energy and environmental transitions. He works closely with international partners and mentors students at the interface of physics, artificial intelligence, and materials for the future of sustainable technologies.

Sossina M. Haile

Northwestern University, USA

Sossina M. Haile is the Walter P. Murphy Professor of Materials Science and Engineering at Northwestern University. Haile's research encompasses materials for sustainable electrochemical energy technologies. Amongst her many awards, in 2008 Haile received an American Competitiveness and Innovation (ACI) Fellowship from the U.S. National Science Foundation, and in 2025 the Sosman Award of the American Ceramics Society. She is a fellow of the Materials Research Society, the American Ceramics Society, the Royal Society of Chemistry, the African Academy of Sciences, and the Ethiopian Academy of Sciences. She is the incoming President of the Materials Research Society and serves on the editorial advisory boards of Joule and MRS Energy & Sustainability.

Ruud van Ommen

Delft University of Technology, Netherlands

Ruud van Ommen is a Professor at Delft University of Technology. He has been a visiting professor at Chalmers University of Technology (Sweden) and the University of Colorado (USA). He has a broad expertise in multiphase reactors and particle technology. Over the past decade, he has expanded his research to include the scalable production of advanced, nanostructured materials. In 2011, he started an ambitious program (funded by an ERC Starting Grant) to investigate the interplay between agglomeration and coating of nanoparticles in the gas phase. This fundamental work has led to practical applications in energy conversion and storage, as well as pharmaceutical production. He is the co-founder of Powall, a spin-off company that works with nanocoating particles.

Kamal Kishore Pant

Indian Institute of Technology Roorkee, India

K.K. Pant is the Director of IIT Roorkee and Professor of Chemical Engineering at IIT Delhi. He holds adjunct and honorary faculty positions at the University of Saskatchewan and the University of Queensland. Prof. Pant's research spans green catalysis and reaction engineering, including coal-to-methanol, e-waste and plastic valorization, hydrogen generation, CO_2 capture and conversion, and biomass valorization to chemicals and fuels. With more than 320 Journal publications, 16 major patents, and over 22,500 citations, Prof. Pant is a well-known researcher across the Globe. Prof. Pant is a fellow of multiple national and international academies such as Indian National Academy of Engineers, National Academy of Sciences, and Royal Society of Chemistry, London.

Daniel M. Kammen

Johns Hopkins University, USA

Daniel M. Kammen is a Professor at Johns Hopkins University, focusing on energy innovation, decarbonization, energy access, and climate justice. He recently served as Senior Advisor for Energy and Innovation at USAID (2021–22). Kammen previously served as the first Environment and Climate Partnership for the Americas (ECPA) Fellow (2010) & as U.S. Science Envoy under Secretary of State John Kerry and President Obama (2016–17). He has founded or serves on the board of over 10 companies & advised the State of California and the U.S. federal government. Kammen was the first Chief Technical Specialist for Renewable Energy and Energy Efficiency at the World Bank (2010–2011) and has contributed to multiple IPCC reports since 1999, with the IPCC sharing the 2007 Nobel Peace Prize.

Vivek Polshettiwar

Tata Institute of Fundamental Research, India

Vivek Polshettiwar is a Professor of Chemistry at TIFR, Mumbai. His research focuses on advanced nanomaterials and nanocatalysis for harvesting solar energy and converting CO_2 into valuable chemicals and fuels, particularly through the use of black gold and defect engineering. He has published nearly 150 research articles and filed 15 patents. He is the recipient of the prestigious ORISE Research Fellowship at the US-EPA and received the Asian Rising Star Lectureship at the 15th Asian Chemical Congress (ACC) in Singapore. Prof. Polshettiwar is a Fellow of the National Academy of Sciences, India; the Indian Academy of Sciences; and the Royal Society of Chemistry, UK. In 2024, he was awarded the Shanti Swarup Bhatnagar Award, India's highest honor in science.

Moses Tade

Curtin University, Australia

Moses Oludayo Tade is the John Curtin Distinguished Professor at Curtin University. Dr. Tade has an extensive leadership and management expertise in higher education across several portfolios for over three decades. He is a visionary and strategic leader; a change agent; mentor and an extensive successful developer of people and the next generation of leaders at various levels. He is a Fellow of the Institution of Chemical Engineers (FIChemE), an Honorary Fellow of Engineers Australia, and a Fellow of the Nigerian Academy of Engineering. He is the Founding Editor-in-Chief of the Asia-Pacific Journal of Chemical Engineering and an international accreditor for IChemE. He has supervised more than 70 Ph.D. students and research fellows.

Josephine Mary Hill

University of Calgary, Canada

Josephine Mary Hill is a Professor in the Department of Chemical and Petroleum Engineering at the University of Calgary's Schulich School of Engineering. She completed her PhD at the University of Wisconsin–Madison and worked at Surface Science Western between her graduate degrees. Her research focuses on catalysis for hydrotreating, gasification, and the conversion of solid waste materials such as petroleum coke and biomass into catalyst supports and activated carbon. She chaired the Canadian Catalysis Division and is President of the Canadian Catalysis Foundation and Past-chair of the Chemical Institute of Canada. Dr. Hill has received numerous awards & fellowships for research & mentoring excellence.

Mark T. Swihart

University at Buffalo, USA

Mark T. Swihart is a SUNY Distinguished Professor in the Department of Chemical and Biological Engineering at the University at Buffalo, where he also served as Department Chair from 2018 to 2024. His research focuses on the synthesis, processing, and applications of nanoparticles and nanomaterials, including pioneering work on silicon nanocrystals for bioimaging and the development of advanced multi-component nanomaterials. Prof. Swihart has authored over 320 papers, co-authored the 8th and 9th editions of Introduction to Chemical Engineering Thermodynamics, and is a Fellow of the American Association for the Advancement of Science and the American Institute of Chemical Engineers.

Muthanna H. Al-Dahhan

Missouri University of Science and Tech., USA

Muthanna Al-Dahhan is the Curators' Distinguished Professor of Chemical and Biochemical Engineering and of Nuclear Engineering and Radiation Science at Missouri University of Science and Technology, where he also holds the Wayne and Gayle Laufer Endowed Chair in Energy. He is an AIChE Fellow, ABET Program Evaluator and incoming ABET Commissioner, and an affiliated professor with Mohammed VI Polytechnic University (UM6P) in Morocco. His research centers on multiphase flow and reactor engineering, including the development of the mFReel laboratory, a globally unique research facility. Dr. Al-Dahhan has authored over 360 publications and supervised more than 150 graduate and postdoctoral researchers.

Krishna Rajan

University at Buffalo, USA

Krishna Rajan is the SUNY Distinguished Professor and the inaugural Erich Bloch Chair of the Department of Materials Design and Innovation at the University at Buffalo: the State University of New York. Professor Rajan is the leading proponent of the field of Materials Informatics. His research is on the application of information science and data-intensive methodologies for the discovery, characterization and modeling of materials. He received his undergraduate education at the University of Toronto and a doctorate from MIT followed by a postdoctoral appointment at Cambridge University; all in the field of Materials Science and Engineering.

Rajagopalan Srinivasan

Indian Institute of Technology Madras, India

Rajagopalan Srinivasan is a Professor of Chemical Engineering at the Indian Institute of Technology Madras, where he leads the American Express Lab for Data Analytics, Risk & Technology (DART Lab), a cross-disciplinary center studying risk and human behavior. He also heads the Intelligence and Applications in Chemical Engineering (IACE) Lab, which develops artificial intelligence and systems engineering methods for the design and resilient operation of complex systems. He obtained his PhD from Purdue University. Before returning to IIT Madras, he served on the faculty at the National University of Singapore and IIT Gandhinagar, where he made significant contributions to process systems and AI-driven engineering research.

Gauri Singh

International Renewable Energy Agency, UAE

Gauri Singh is the Deputy Director-General of the International Renewable Energy Agency (IRENA), bringing over 30 years of experience in renewable energy policy, advocacy, and sustainable development. She previously served at senior levels in India's federal and state governments, where she led the development of India's National Solar Mission in 2010 and guided major rural development and poverty-reduction initiatives in Madhya Pradesh. At IRENA, she earlier served as Director of Country Support and Partnerships, leading regional initiatives and partnerships with energy and economic organizations. Her work continues to shape global strategies for renewable energy deployment and sustainable transitions.

Rangan Banerjee

Indian Institute of Technology Delhi, India

Rangan Banerjee is the Director of the Indian Institute of Technology Delhi and a Professor in the Department of Energy Science and Engineering at IIT Bombay, where he previously served as the founding head of the department. He holds the Forbes Marshall Chair in Energy and has led major national initiatives in energy systems, hydrogen technologies, and sustainable energy planning. Prof. Banerjee has been a key advisor to India's energy agencies and has contributed to policy development in renewables, energy security, and low-carbon transitions. He received his B.Tech. and Ph.D. from IIT Bombay and has published extensively in the fields of energy systems modeling and energy policy.

Lourdes Vega

Khalifa University, UAE

Lourdes F. Vega is a Full Professor of Chemical Engineering and the Founder/Director of the Research and Innovation Center on CO_2 and Hydrogen (RICH Center) at Khalifa University, where she leads major initiatives in clean energy, CCUS, hydrogen, and sustainable fuels. Her research integrates experimental methods with computational modeling, machine learning, and molecular thermodynamics to advance CCU, H_2 production, storage and utilization, sustainable fuels, cooling technologies, and water treatment. She has authored 320+ publications, holds 8 patents, and received honors including the Mohammed Bin Rashid Medal for Scientific Achievement, recognition among Spain's TOP100 Women Leaders, V60 Women in the Middle East, and Global 50 Women on Hydrogen 2025.

Alex Aliper

Insilico Medicine, UAE

Alex Aliper, Ph.D., 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. He 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, and he has published over 50 peer-reviewed publications. He was recognized as one of the "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.

Safiya Khalil Al Hashmi

New York University Abu Dhabi, UAE

Safiya Al Hashmi is an Assistant Professor Emerging Scholar of Mechanical Engineering at NYU Abu Dhabi. She earned her Ph.D. in Chemical and Biomolecular Engineering from Rice University in 2023. She currently leads the Khalil Research Group, which leverages a cross-disciplinary approach that merges chemistry, reaction engineering, and manufacturing principles to design materials for applications in the water and energy sectors. Dr. Al Hashmi is a co-investigator of the Center for Smart Engineering Materials (CSEM) and the Center for Quantum and Topological Systems (CQTS). She is a recipient of the 2024 NYU Research Catalyst Grant and was named one of MIT Technology Review Innovators Under 35 in the Middle East for 2024.

Johannes Hachmann

University at Buffalo, USA

Johannes Hachmann is an Associate Professor in the Department of Chemical & Biological Engineering at the University at Buffalo. He obtained his Ph.D. in Theoretical Chemistry from Cornell University and completed postdoctoral research at Harvard University before joining UB. His research focuses on computational chemistry, computational materials science, and applied data science, using quantum chemical modeling, high-throughput screening, ML, and materials informatics to design molecules, materials, and catalysts. His work has been recognized with several prestigious awards, including the RSC Scholarship Award for Scientific Excellence of ACS CINF, IBM-Löwdin Award, IBM-Zerner Award, and the SCES Young Investigator Award.

Tarak Karmakar

Indian Institute of Technology Delhi, India

Tarak Karmakar is an Associate Professor in the Department of Chemistry at the Indian Institute of Technology Delhi. He joined the institute as a faculty member in June 2021 and was promoted to Associate Professor in July 2025. He received his Ph.D. from the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bengaluru, in 2017, followed by postdoctoral research from 2017 to 2021 at ETH Zurich, USI Lugano, and IIT Genova. At IIT Delhi, his research focuses on the development of advanced enhanced-sampling methodologies, machine-learning interatomic potentials, and data-driven modelling frameworks to unravel nano–bio interactions, study catalytic processes, and investigate complex biomolecular mechanisms.

Mani Bhushan

Indian Institute of Technology Bombay, India

Mani Bhushan is a Professor in the Department of Chemical Engineering at IIT Bombay, where he has served since 2005. He is also associate faculty at Centre of Machine Intelligence and Data Science (CMInDS) at IIT Bombay. He received his B.Tech (1997) and Ph.D. (2001) from IIT Bombay, followed by a postdoctoral appointment at Purdue University (2001–2002) and an Assistant Professorship at the University of Alberta (2003–2005). His research spans optimal sensor placement, state and parameter estimation, fault detection and diagnosis, and data analytics. He works on graph-based sensor network design and audit, nonlinear state and parameter estimation, and data-driven applications in renewable energy and pollution source identification.

Sriganesh Karur

Ex-General Manager, Shell

Sriganesh Karur is a chemical engineer and digital transformation leader with over 30 years of experience in refining, petrochemicals, process modeling, and advanced optimization. He earned his B.Tech in Chemical Engineering from BITS Pilani and a Doctorate from Washington University in St. Louis, specializing in numerical methods for reaction engineering. Dr. Karur has held global roles at Aspen Technology and Shell, implementing real-time optimization, advanced process control, and digital solutions to enhance industrial reliability and efficiency. He is the Founder and President of InspiraLux LLC, an independent consulting practice focused on engineering leadership and sustainable digital transformation.

Vivek Buwa

Indian Institute of Technology Delhi, India

Vivek V. Buwa is the Schlumberger Chair Professor in the Department of Chemical Engineering at IIT Delhi, where he also serves as the Deputy Director (Strategy and Planning). He obtained his doctorate jointly from IIT Bombay and CSIR's National Chemical Laboratory Pune. His research interests include computational flow modelling and simulation, transport phenomena and reactions in multiphase systems and process intensification. He joined IIT Delhi in 2006 as an Assistant Professor and was promoted to Full Professor in 2017. He is a recipient of research fellowships from the Bavarian Science Foundation and the Alexander von Humboldt Foundation, Young Engineer Award from the Indian National Academy of Engineering and Teaching Excellence Award from IIT Delhi.

Ankur Gupta

University of Colorado, USA

Ankur Gupta is an Assistant Professor in the Department of Chemical and Biological Engineering at the University of Colorado, Boulder. He serves as the principal investigator of the Laboratory of Interfaces, Flow, and Electrokinetics (LIFE). His research interests include interfacial phenomena, complex fluids, multiphase flows, and diffusiophoresis, with a focus on their applications in the physics of life, energy storage, desalination, and lab-on-a-chip technologies. Dr. Gupta's work has been featured in over 150 news outlets, including The New York Times, CNN, and The Print, and he has received several honors, including C&EN Talented 12, the Johannes Lyklema Early Career Award, AIChE 35 Under 35, the NSF CAREER Award, and IIT Delhi's GOLD Award.

Bijay Tripathi

Indian Institute of Technology Delhi, India

Bijay P. Tripathi is an Associate Professor in the Department of Materials Science and Engineering at IIT Delhi. He obtained his Ph.D. from CSIR–CSMCRI, Bhavnagar, and subsequently worked at the Leibniz Institute of Polymer Research, Germany as an Alexander von Humboldt postdoctoral fellow before starting his independent career at IIT Delhi. He has received several prestigious fellowships, including DAAD, Alexander von Humboldt, JSPS, Marie Curie, INSA young scientist, etc. His research focuses on the synthesis of polymers and nanomaterials, surface functionalization, and the development of nanoporous and charged membranes and nanocatalysts for applications in energy, water, separations, catalysis, and environmental remediation.

Husain Kanchwala

Indian Institute of Technology Delhi, India

Husain Kanchwala is an Assistant Professor in the Center of Automotive Engineering and Tribology at IIT Delhi, specializing in vehicle system dynamics and control, with broader interests in dynamical systems. His research integrates modeling, simulation, and advanced control strategies to improve vehicle performance, safety, and stability. He has worked in diverse, multidisciplinary research environments, collaborating with leading international institutions such as the University of Queensland, NYCU Taiwan, University of Warwick, KTH Royal Institute of Technology, and the University of Seville. In addition to academia, he has industry experience at Mahindra & Mahindra (R&D, Mumbai), where he contributed to applied research & real-world engineering solutions.

Chithirai Pon Selvan

Curtin University Dubai, UAE

Chithirai Pon Selvan is the Director of Research and Head of the School of Science & Engineering at Curtin University Dubai. His research spans machine design, optimization techniques, advanced manufacturing, renewable energy, and sustainable engineering development. He has published over 150 research articles and has authored or edited several books. He is a member of several professional societies including SAE, ASHRAE, IMechE, ASME, EI, ASQ, IEEE, and ISTE, and is a Senior Fellow of the Higher Education Academy (SFHEA), UK. He has received multiple awards including the Teaching Excellence Award, the Dubai Award for Sustainable Transport, Dr. Kalam's International Excellence Award, and the Distinguished Conservation Project Award.

Suddhasatwa Basu

Indian Institute of Technology Delhi, India

Suddhasatwa Basu holds Federation of Indian Petroleum Industry (FIPI) Chair Professor on Clean Energy at IIT Delhi. He is the former Director of CSIR-Institute of Minerals & Materials Technology, Bhubaneswar. He has extensive experience in developing materials for energy conversion and storage, including green hydrogen and fuel cell technologies, rechargeable batteries, electrosynthesis, and waste-to-wealth processes for a circular economy. He has published over 290 articles, holds 16 patents with two transferred technologies, is a Fellow of INSA, NASI, INAE, and the RSC (UK), and has received honors including the Fulbright Fellowship, Herdillia Award, Dr. A. V. Rama Rao Foundation Research Award, SMC Gold Medal, and the MRSI Medal.

Abhijit Chatterjee

Indian Institute of Technology Bombay, India

Abhijit Chatterjee is a Professor in the Department of Chemical Engineering at IIT Bombay. His research spans materials modeling for energy applications, process systems engineering, sustainability, and multiscale simulations, with a strong focus on energy and climate. He uses advanced computational techniques, including density functional theory, molecular dynamics, and Monte Carlo methods to investigate materials for green energy and environmentally friendly technologies. He has received several notable honors, including awards from the Indian National Academy of Sciences (INSA) and the National Academy of Sciences India (NASI). His work effectively bridges fundamental science with practical innovations in sustainable energy and advanced materials.

Sivaprakash Sengodan

Khalifa University, UAE

Sivaprakash Sengodan is an Assistant Professor in Mechanical Engineering at Khalifa University (UAE). Previously, he was an Imperial College Research Fellow (ICRF) in the Department of Materials at Imperial College London, and he holds a Ph.D. in Energy Engineering from Ulsan National Institute of Science and Technology, South Korea (2015). Dr. Sengodan's research focuses on understanding key ionic and electronic transport processes in electrochemical devices, including electrolyzers, membranes, and fuel cells. He utilizes isotopic labeling experiments to study protonic and oxygen ion diffusion in ceramics, in combination with X-ray and neutron scattering approaches, to enable the correlation of functional performance with structural evolution.

Ahsan Qurashi

Khalifa University, UAE

Ahsan Qurashi is an Associate Professor of Chemistry at Khalifa University. He earned his Ph.D. from Chonbuk National University, South Korea, and completed postdoctoral research at Toyama University, Japan under the VBL program. He previously served as Assistant and Associate Professor at King Fahd University of Petroleum and Minerals, Saudi Arabia. He has supervised several undergraduate, Masters, and PhD students in strategic research areas. His research focuses on developing new materials, clean energy generation and storage, catalysis, sensors, and biomedical applications. He also serves on the editorial boards of the International Journal of Hydrogen Energy, Materials Research Bulletin, and Scientific Reports.

Anil Verma

Indian Institute of Technology Delhi, India

Anil Verma is the Dean International Programmes, and a Professor in the Department of Chemical Engineering at IIT Delhi. His research focuses on sustainable electrochemical systems, including redox flow batteries, fuel cells, CO_2 electrochemical reduction, aluminum-ion batteries, graphene synthesis, and C/C composites. He leads the Sustainable Environergy Research Lab (SERL) and heads the DST–IITD Centre for Energy Storage Platform on Batteries (ESPOB). He has published over 120 research articles, filed multiple patents, and supervised numerous Ph.D. students. He has also served as a Visiting Professor at Washington University in St. Louis and a Visiting Fellow at Newcastle University (United Kingdom).

Ananth Govind Rajan

Indian Institute of Science Bengaluru, India

Ananth Govind Rajan is an Associate Professor of Chemical Engineering at the Indian Institute of Science, Bengaluru, specializing in the modeling and simulation of nanomaterials for clean energy and water technologies. His research focuses on understanding structure–property relationships at the nanoscale to design materials with improved performance and sustainability. He has received several notable honors, including the Prof. Priti Shankar Teaching Award and the Infosys Young Investigator Award, and has been recognized as an Influential Researcher by Industrial & Engineering Chemistry Research. He also contributes to the research community through service on the Early Career Boards of Nano Letters and EES Catalysis.

Maryam Khaleel

Khalifa University, UAE

Maryam Khaleel obtained her Ph.D. from the University of Minnesota (USA) in 2015 and is currently an Associate Professor of Chemical Engineering at Khalifa University, specializing in the development of porous materials to accelerate the global transition to clean energy, with breakthroughs in additive-free synthesis of hierarchical materials and the discovery of new structural mechanisms governing their formation. The materials she develops enable sustainable catalysis to produce clean fuels and chemicals, carbon utilization, and next-generation energy storage. Her achievements have been recognized through the L'Oréal-UNESCO For Women in Science Fellowship, the SWARD Award by Sandooq Alwatan, and the Sheikh Rashid Award for Scientific Achievement.

Suprakas Sinha Ray

DSI-CSIR, South Africa

Suprakas Sinha Ray completed his PhD at the University of Calcutta in 2001 and later conducted postdoctoral research at the Toyota Technological Institute and Laval University, where he worked on nanoclay–polymer nanocomposites. He joined Council of Scientific and Industrial Research (CSIR) as a group leader, focusing on both the fundamental understanding and real-world applications of polymer-based nanostructured materials. He subsequently rose to Chief Researcher (Level III, the highest SET position in CSIR) and became Director of the DSI-CSIR Nanotechnology Innovation Centre. Under his leadership, the Centre has expanded into a globally recognized hub, fostering collaborations among scientists, engineers, postdoctoral researchers, students, & industry partners.

Manjesh Kumar

Indian Institute of Technology Delhi, India

Manjesh Kumar, a Professor at IIT Delhi, focuses on the optimal design of zeolite catalysts with enhanced physicochemical properties. His research investigates zeolite growth mechanisms and applies this knowledge to tailor crystal size and morphology using commercially viable modifiers. He increasingly employs advanced in situ AFM techniques to gain deeper insight into nanoscale growth processes, enabling the development of superior catalytic materials. Alongside his academic work, he brings valuable industrial experience from his tenure as a project and production manager at Ranbaxy Laboratories. He also remains active in professional outreach and community engagement through his involvement with IITAGH.

Dinesh Shetty

Khalifa University, UAE

Dinesh Shetty is an Associate Professor of Chemistry at Khalifa University, UAE. Dr. Shetty was selected to be featured as an innovator at Land of Dreamers Who Do at the UAE Pavilion of Dubai Expo 2020. Recently, he was awarded the US National Academy of Science Arab-American Frontiers Award and Sharjah Sustainability Award. He has authored over 90 research articles, over 45 conference papers, delivered more than 45 invited talks, and holds 9 US 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.

Dibyajyoti Ghosh

Indian Institute of Technology Delhi, India

Dibyajyoti Ghosh is an Assistant Professor at IIT Delhi, where he holds a joint appointment in the Department of Materials Science and Engineering and the Department of Chemistry. He earned his Ph.D. from JNCASR, Bangalore, and brings extensive international experience from his postdoctoral tenures at the University of Bath, UK, and Los Alamos National Laboratory (LANL), USA. He leads the "Computational Design of Functional Materials" (CDFM) research group, focusing on the intersection of computational chemistry, condensed matter physics, and data science. His research expertise lies in DFT, non-adiabatic molecular dynamics, and machine learning to design novel materials for optoelectronics, solar cells, and photocatalysis.

Dan Sun

Queen's University Belfast, UK

Dan Sun is an Associate Professor in Advanced Composite Research at Queen's University Belfast. Her research work focuses on developing innovative composite materials and advanced manufacturing techniques for engineering applications. She specializes in composite science and advanced manufacturing and has received the Royal Academy of Engineering & Leverhulme Trust Fellowship for 2025/26. Her research has been supported by funding bodies including UKRI, the Royal Society, EU Horizon 2020, and the Qatar National Research Fund (QNRF). She has published over 100 peer-reviewed journal articles, accumulating more than 5,000 citations, with an H-index of 46. Dr. Sun is also a Chartered Engineer and a member of several professional organizations.

Martin Takáč

Mohamed Bin Zayed University of AI, UAE

Martin Takáč is an Associate Professor and Associate Department Chair in the Machine Learning Department at MBZUAI. His work focuses on designing and analyzing algorithms for ML, AI-driven scientific discovery, and applications in energy systems and protein-DNA interaction studies. Before joining MBZUAI, he was an Associate Professor in Industrial and Systems Engineering at Lehigh University. His research has been recognized with several awards, including the OR Society Best Ph.D. Dissertation Award (2014), the Leslie Fox Prize (2nd Prize, 2013), and the Charles Broyden Prize (2022). He has received funding from multiple NSF programs and collaborated on several grants with the Weizmann Institute of Science.

Sergey Kozlov

National University of Singapore, Singapore

Sergey M. Kozlov is an Assistant Professor at NUS where he leads the Computational Nanocatalysis group, which performs multi-disciplinary research at the crossroads of chemical engineering, theoretical chemistry, and nanoscience. His research focuses on DFT, nanostructured materials, and the computational design of systems for catalysis and electrochemistry. He has significant expertise in heterogeneous catalysis, graphene, and the advanced modeling of complex nanomaterials. His work contributes to the design of more efficient, sustainable, and technologically relevant materials for energy and environmental applications. He was awarded fellowship by the National Research Foundation (Singapore) for studies of metal-oxide interactions in catalysis.

Vikram Singh

Indian Institute of Technology Delhi, India

Vikram Singh is an Associate Professor in the Department of Chemical Engineering at IIT Delhi. His research focuses on colloids, emulsions, and aerosols, with current interests spanning air pollution in the Indo-Gangetic Plain, real-time chemical speciation and source apportionment of particulate matter, light scattering in emulsions and aerosol suspensions, and CO_2 capture and utilization for metal extraction and sequestration in demolition waste. A chemical engineer by training, Dr. Singh earned his B.Tech. from IIT Delhi and his MS and Ph.D. from Cornell University. Prior to joining IIT Delhi, he worked as a Research Engineer at ConocoPhillips and Phillips 66, and as a Postdoctoral Fellow in the Department of Seismology at Columbia University.

Nirpendra Singh

Khalifa University, UAE

Nirpendra Singh is an Associate Professor at Khalifa University, UAE. Before joining Khalifa University, he held research positions as a scientist at KAUST, Saudi Arabia, and as a research professor at the Sungkyunkwan University, South Korea. Dr. Singh's research focuses on discovering novel van der Waals layered materials and their heterostructures through advanced computational methods and algorithms. His group investigates the electronic, magnetic, thermal transport, and catalytic properties of 2D materials, with applications spanning valleytronics, thermoelectrics, and sustainable energy technologies. He has published more than 100 peer-reviewed articles in leading journal and has received the Faculty Scholarship Excellence Award: Innovation Excellence (2024).

Ejaz Ahmad

IIT (ISM) Dhanbad, India

Ejaz Ahmad is a faculty member in the Department of Chemical Engineering at IIT (ISM) Dhanbad, Head of the Naresh Vashisht Centre for Hydrogen and CCUS Technologies, and Faculty In-Charge of Sponsored Research & Industrial Consultancy. He is a two-time recipient of India's Gandhian Young Technological Innovation Award (GYTI). His research focuses on heterogeneous catalysis for biorenewable energy, green gasoline, sustainable aviation fuel, clean hydrogen, waste-to-wealth, and urban mining. He has also received the DAAD Bi-national Research Grant and works on coal characterization and conversion, biofuels, hydrogen production, carbon dioxide capture, and metal recovery from e-waste and batteries.

Divya Nayar

Indian Institute of Technology Delhi, India

Divya Nayar is an Associate Professor at the Department of Materials Science and Engineering at IIT Delhi. She completed her Ph.D. in Computational Chemistry at IIT Delhi. She conducted postdoctoral research at TU Darmstadt, Germany, and previously served as Assistant Professor at IIT Kharagpur's Centre for Computational and Data Sciences. Her research focuses on soft matter simulations, biomolecular self-assembly, and solvation using molecular dynamics, statistical mechanics, and thermodynamic theories. She applies these insights to design bio-inspired nanomaterials with tailored properties for advanced applications. Her work has earned several recognitions, the most notable being her selection as an Associate of the Indian Academy of Sciences.

Ashutosh Yadav

Indian Institute of Technology Jammu, India

Ashutosh Yadav is a faculty member in the Department of Chemical Engineering at IIT Jammu. He previously worked as a Senior Research Scientist at Bharat Petroleum Corporation's Corporate R&D Centre in Greater Noida from 2017 to 2020. His research spans multiphase reactors, computational fluid dynamics, process optimization, petroleum refining, and environmental engineering. He integrates machine learning and advanced modeling tools to enhance process efficiency and sustainability across chemical and energy systems. His teaching interests include Data Science for Chemical Engineers, Chemical Reaction Engineering, Chemical Engineering Thermodynamics, and Petroleum Refinery and Petrochemicals, reflecting his broad technical expertise.

Munawar A. Shaik

United Arab Emirates University, UAE

Munawar A. Shaik is an Associate Professor at UAE University, Al Ain, with a PhD in Chemical Engineering from IIT Bombay (2005). He has over 20 years of experience in modeling, optimization, and process systems engineering, including planning, scheduling, and supply chain management. He served as Assistant and Associate Professor at IIT Delhi and was on sabbatical at Petroleum Institute, Khalifa University, Abu Dhabi. His research focuses on process operations, synthesis, heat and water networks, energy technologies, and evolutionary computation. He combines theoretical and computational approaches to optimize chemical and energy processes for industrial and environmental applications.

Jayaram Valluru

Indian Institute of Technology Ropar, India

Jayaram Valluru is a faculty member in the Department of Chemical Engineering at IIT Ropar. His research focuses on Process Systems Engineering, including Bayesian state and parameter estimation, soft-sensing, data reconciliation, and fault detection using first-principles and ML approaches. He has experience in developing integrated Model Predictive Control and Real-Time Optimization frameworks for large-scale chemical processes. His current work explores hybrid estimation algorithms that integrate process knowledge with big data techniques for plant-wide soft-sensing and data reconciliation. Future research includes intelligent control frameworks for continuous and batch processes using advanced ML methods for industrial applications.

Nitesh Kumar

Indian Institute of Technology Jammu, India

Nitesh Kumar is an Assistant Professor at the Indian Institute of Technology Jammu, where he works at the cutting edge of materials design for Energy and Biomedical Applications. His research interests are primarily focused on metal hydrides, metal polymer composites, and soft polymeric materials. His work is pivotal in developing next-generation materials for hydrogen energy, chronic wound healing and materials for sustained drug release. By investigating the fundamental principles of hydrogen-material interaction, his work is focused on finding next-generation materials for sustainable and safe hydrogen storage and delivery, thereby reducing the global carbon footprint.

Manoj Ramteke

Indian Institute of Technology Delhi, India

Manojkumar Ramteke is a Professor in the Department of Chemical Engineering at IIT Delhi. He is a distinguished figure in the field of Process Systems Engineering, known for his innovative application of AI to industrial challenges. His research interests focus on the development and application of Evolutionary Algorithms, ML, and meta-heuristic techniques for the optimization, planning, and scheduling of complex chemical processes. His work aims to enhance operational efficiency and sustainability in the chemical industry by integrating data-driven decision-making with traditional engineering principles. He has authored numerous high-impact papers, cementing his reputation as a leader in computational chemical engineering.

Shelaka Gupta

Indian Institute of Technology Hyderabad, India

Shelaka Gupta is an Assistant Professor in the Department of Chemical Engineering at the IIT Hyderabad. Her research employs a synergistic approach, combining experimental kinetic studies with atomistic simulations to design robust catalysts for sustainable energy applications. Dr. Gupta focuses on critical areas, including biomass valorization, methane upgradation, and design of multi-component alloys. She has been recognized as India's 75 women in STEM by the Office of Principal Scientific Adviser to the Government of India. She has received the Sumant Sinha Sustainability Leadership Award (2019) and Gandhian Young Technological Innovation (GYTI) Award (2018) and is also an entrepreneur and co-founder of WowChemE Pvt Ltd.

Om Prakash

Indian Institute of Technology Delhi, India

Om Prakash is an Assistant Professor in the Department of Chemical Engineering at IIT Delhi. His research lies at the intersection of Process Systems Engineering and Data Science, focusing on the digitalization of the chemical industry (Industry 4.0). Dr. Prakash specializes in the development of Machine Learning algorithms, graph analytics, and dynamic modeling techniques for process monitoring and fault diagnosis. His work addresses the complexities of sensor placement design, networked systems, and the optimization of large-scale processes. By developing advanced data-driven strategies, he aims to enhance the safety, reliability, and operational efficiency of chemical plants, ensuring they meet modern standards of automation and smart manufacturing.

Rajesh Kumar Upadhyay

IIT (BHU) Varanasi, India

Rajesh Kumar Upadhyay is a Professor in the Department of Chemical Engineering at IIT (BHU) Varanasi. He is a highly respected researcher in the domain of Chemical Reaction Engineering and Multiphase Flow. Prof. Upadhyay is particularly renowned for his expertise in non-invasive flow monitoring techniques. His diverse research portfolio covers hydrogen production via membrane reformers, catalyst development, and waste-to-energy technologies. He has led numerous high-value research projects aimed at designing efficient industrial reactors and sustainable energy systems. Prof. Upadhyay's work provides critical insights into reactor hydrodynamics, facilitating the scale-up and optimization of complex chemical processes.

Deepak Kumar

Indian Institute of Technology Delhi, India

Deepak Kumar is an Assistant Professor in the Department of Physics at IIT Delhi. His research is deeply rooted in experimental soft matter physics, where he investigates the mechanics and dynamics of complex systems. Dr. Kumar focuses on a variety of phenomena, including the rheology of granular materials, the impact dynamics of fluid drops, and the elasto-capillarity of thin sheets. His work often explores the physics of everyday occurrences to uncover fundamental principles that have broad applications in material science and industry. Recently, his research has expanded to include the development of "liquid marbles" and novel encapsulation techniques using thin polymer films, with potential in drug delivery, micro-reactors, and controlled wetting technologies.

Vinay Gupta

Khalifa University, UAE

Vinay Gupta is an Assistant Professor in the Department of Physics at Khalifa University, UAE. He is a distinguished materials scientist and a recipient of the prestigious Shanti Swarup Bhatnagar Prize (2017) for his outstanding contributions to the physical sciences. Dr. Gupta's research interests lie in the development of organic and hybrid materials for energy harvesting and storage devices, including organic solar cells, supercapacitors, and lithium-ion batteries. He has pioneered work in the area of conducting polymers and carbon nanotube arrays. At Khalifa University, he continues to push the boundaries of flexible electronics and sustainable energy technologies, focusing on creating efficient, low-cost materials for a green energy future.

Madhulika Gupta

IIT (ISM) Dhanbad, India

Madhulika Gupta is an Assistant Professor in the Department of Chemistry and Chemical Biology at the IIT (ISM) Dhanbad. Her research expertise is centered on Computational Chemistry and Biophysics, where she utilizes high-performance computing to solve complex biological and chemical problems. Dr. Gupta employs MD simulations and quantum chemical calculations to investigate protein-protein interactions, enzyme mechanisms, and biomolecular recognition processes. Her work advances computer-aided drug discovery and the design of catalysts for biomass conversion, providing atomistic insights that support the development of novel therapeutics and efficient catalytic systems for renewable energy.

Rachit Khare

Technical University of Munich, Germany

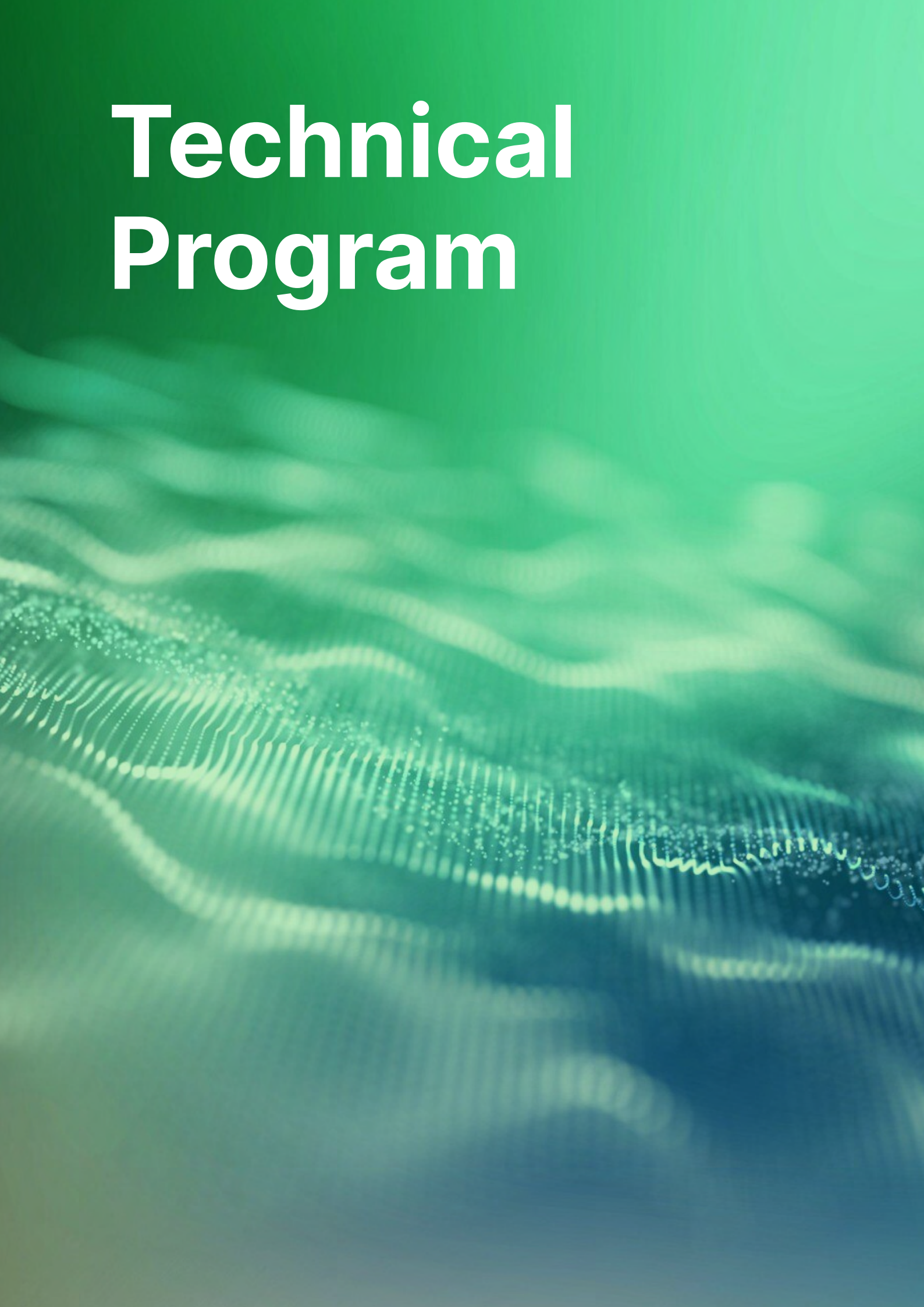
Rachit Khare is a Group Leader at the Chair of Technical Chemistry II at the Technical University of Munich (TUM), Germany. He earned his Ph.D. from the University of Minnesota, specializing in heterogeneous catalysis and reaction kinetics. His research combines operando X-ray absorption spectroscopy with molecular simulations to unravel structure-function relationships. Dr. Khare focuses on designing robust catalytic systems for sustainable energy applications, including photochemical/electrochemical processes and plastic upcycling using ionic liquids. His work bridges fundamental mechanistic understanding with practical catalyst design, contributing to the development of efficient and environmentally sustainable chemical technologies.

Shivraj Karewar

Technology Innovation Institute, UAE

Shivraj Karewar is a Senior Researcher at the Technology Innovation Institute (TII) in Abu Dhabi, UAE, specializing in computational materials science. His work integrates advanced atomistic simulations and machine learning to accelerate the design and discovery of next-generation materials. His research bridges fundamental theory with real-world applications, enabling data-driven development of high-performance materials for critical technologies. He currently leads efforts in predictive modeling, materials design, and optimization. With a strong record of international collaboration across Europe and the United States, Dr. Karewar has contributed to advancements that significantly reduce the time and cost of traditional experimental workflows, supporting a more efficient, simulation-guided approach to materials innovation.

Technical Program



Sunday, 14th December 2025		
Time	**Venue: IIT Delhi - Abu Dhabi, Khalifa City B, Abu Dhabi (Entry from Gate 6 or 7)**	
11:30 - 12:30	**Registration and Lunch**	
12:30 – 14:30	**Workshop 1** **Hands-on with Data-Driven Approaches to Accelerate Catalysis and Materials Research** *(Meta)* **Zachary W. Ullissi** Meta Fundamental AI Research **Rachit Khare** Technical University of Munich	**Workshop 2** **Why High-Quality Presentations and Posters Matter?** *(American Chemical Society)* **Ajay Jha** Assistant Director, ACS Publications
14:30 - 15:00	**Coffee Break and Campus Tour**	
15:00 – 17:00	**Workshop 3** **Innovation & Lab-to-Industry Pathways** *(American Chemical Society)* **Ajay Jha** Assistant Director, ACS Publications	**Workshop 4** **Research Data Management for Catalysis and Materials Research** *(NFDI4Cat and SPARC)* **Michael Libeau** University of Leipzig **Mohammad Khatamirad** Technical University of Berlin **Nikolaos G. Moustakas** Leibniz Institute for Catalysis **Rachit Khare** Technical University of Munich

Monday, 15th December 2025					
Time	**Venue: Fairmont Bab Al Bahr, Abu Dhabi**				
08:00 - 09:00	**Registration and Coffee**				
09:00 – 09:30	Welcome				
	Distinguished Speakers Session 1 **Venue:** *Saqr Ballroom* **Chairs**: Joseph Smith, Shobhana Narasimhan				
09:30 – 10:00	*Powering the Change - Materials and Processes for Energy Transition* **Johannes A. Lercher**, Technical University of Munich				
10:00 – 10:30	*Multiscale Modeling for Accelerating Carbon Capture and Beyond* **Ahmed Al Hajaj**, Khalifa University				
10:30 – 11:00	**Coffee Break and Poster Session 1**				
	Distinguished Speakers Session 2 **Venue:** *Saqr Ballroom* **Chairs**: Safiya Khalil Al Hashmi, Mark T. Swihart				
11:00 – 11:30	*The Prospect of AI for Materials Discovery and Design of New Energy Materials* **Jeffrey Snyder**, Northwestern University				
11:30 – 12:00	*LIGHT, ELECTRONS and ACTION* **Vivek Polshettiwar**, Tata Institute of Fundamental Research				
12:00 – 12:30	*AI for Science and Sustainability: A Journey from Process Systems Engineering* **Fengqi You**, Cornell University				
12:30 - 13:30	**Group Photo and Lunch**				
	Distinguished Speakers Session 3 **Venue**: *Saqr Ballroom* **Chairs**: Ahmed Al Hajaj, Xiaonan Wang				
13:30 – 14:00	*TBD* **Maryam Al Nahyan**, New York University Abu Dhabi				
14:00 – 14:30	*Nature-Inspired Engineering of Functional Materials via a Systematic Design Methodology* **Marc-Olivier Coppens**, University College London				
14:30 – 15:00	*Discovering Reaction Networks and Life Cycle Pathways for a Sustainable Circular Economy of Chemicals* **Bhavik Bakshi**, Arizona State University				
15:00 – 15:30	*Hybrid Energy Systems: Innovative Research Pathways for Alleviating Global Energy Poverty* **Joseph Smith**, Missouri University of Science & Technology				
15:30 - 16:00	**Coffee Break and Poster Session 1**				
16:00 – 18:00	**Parallel Session 1** ***AI for Sustainable Chemical Processes*** **Venue:** Saqr Ballroom 1	**Parallel Session 2** ***Process Intensification for Sustainability*** **Venue:** Saqr Ballroom 2	**Parallel Session 3** ***Sustainable Materials for Energy Storage*** **Venue:** Saqr Ballroom 3	**YRS Session 1** ***AI & ML for Sustainability*** **Venue:** Al Reem	**Lightning Session 1** **Venue:** Sir Banyas
18:30 - 20:00	**Grand Dinner Reception (Shangri-La Hotel & Resorts, Abu Dhabi)**				

Tuesday, 16th December 2025					
Time	**Venue: Fairmont Bab Al Bahr, Abu Dhabi**				
07:30 - 08:00	**Coffee and Snacks**				
	Distinguished Speakers Session 4 **Venue**: *Saqr Ballroom* **Chairs**: Johannes Hachmann, Moses Tade				
08:00 – 08:30	*Energy Security: Molecular Insight to Industrial Impact. Bringing Speed and Scale to Science for Sustainability* **Ramakrishna R. Sonde**, BITS Pilani, Goa Campus				
08:30 – 09:00	*ML Guided Catalyst Discovery for the Direct Hydrogenation of CO_2 to Jet Fuel* **Jorge Gascon**, King Abdullah University of Science and Technology				
09:00 – 09:30	*Designing Materials for Sustainability from First Principles* **Shobhana Narasimhan**, Jawaharlal Nehru Center for Advanced Scientific Research				
09:30 – 10:00	*2D Nanocomposite Membrane Engineering: A Journey from Research to Production* **Hassan Arafat**, Khalifa University				
10:00 - 10:30	**Coffee Break and Poster Session 2**				
	Distinguished Speakers Session 5 **Venue**: *Saqr Ballroom* **Chairs:** Marc-Olivier Coppens, Josephine Mary Hill				
10:30 – 11:00	*Machine Learning Models Across Chemistry and Materials* **Zachary W. Ulissi**, Meta Fundamental AI Research				
11:00 – 11:30	*Fathoming the Complexities of Reactions at Solid-Liquid Interfaces* **David Flaherty**, Georgia Institute of Technology				
11:30 – 12:00	*AI for Sustainability: Foundation Models for Closed-Loop, Knowledge-Driven Chemical Discovery and Process Optimization* **Xiaonan Wang**, Tsinghua University				
12:00 – 12:30	*Materials for Energy from Advanced Modeling* **Marco Saitta**, Université Pierre et Marie Curie - Sorbonne				
12:30 - 13:30	**Lunch**				
	Distinguished Speakers Session 6 **Venue**: *Saqr Ballroom* **Chairs**: Jeffrey Snyder, Maryam Khaleel				
13:30 – 14:00	*Protonic Ceramic Electrochemical Cells: Status and Outlook* **Sossina M. Haile**, Northwestern University				
14:00 – 14:30	*Scalable Production of Nanostructured Materials for Energy and Health Applications using Gas Phase Deposition* **Ruud van Ommen**, Delft University of Technology				
14:30 – 15:00	*AI for Materials Driven Innovation for a Regenerative Economy* **Krishna Rajan**, University at Buffalo				
15:00 - 15:30	**Coffee Break and Poster Session 2**				
15:30 – 17:30	**Parallel Session 4** ***Materials for Sustainability I*** **Venue:** Saqr Ballroom 1	**Parallel Session 5** ***Carbon Capture and Beyond*** **Venue:** Saqr Ballroom 2	**Parallel Session 6** ***AI for Sustainability I*** **Venue:** Saqr Ballroom 3	**YRS Session 2** ***Materials for Sustainability*** **Venue:** Al Reem	**Lightning Session 2** **Venue:** Sir Banyas
18:00 - 20:00	**Gala Dinner and Musical Night at Fairmont Bab Al Bahr**				

Wednesday, 17th December 2025

Time	Venue: Fairmont Bab Al Bahr, Abu Dhabi				
07:30 - 08:00	**Coffee and Snacks**				
08:00 – 10:00	**Parallel Session 7** ***Sustainable Chem-ical Processes*** **Venue:** Saqr Ballroom 1	**Parallel Session 8** ***AI for Sustainability II*** **Venue:** Saqr Ballroom 2	**Parallel Session 9** ***Materials for Sustainability II*** **Venue:** Saqr Ballroom 3	**YRS Session 3** ***Catalysis and Carbon Capture*** **Venue:** Al Reem	**YRS Session 4** ***Water-Energy-Climate*** **Venue:** Sir Banyas
10:00 - 10:30	**Coffee Break and Poster Session 3**				
	Distinguished Speakers Session 7 **Venue**: *Saqr Ballroom* **Chairs**: Ruud van Ommen, Krishna Rajan				
10:30 – 11:00	*Materials Science and Systems Innovation for the Just Energy Transition* **Daniel M. Kammen**, Johns Hopkins University				
11:00 – 11:30	*Decarbonising the Future: CCU and Hydrogen Landmark Redefining the Future of Energy* **Kamal K. Pant**, Indian Institute of Technology Roorkee				
11:30 – 12:00	*Decarbonising Heavy Industries: The Roles of Carbon Capture and Hydrate-Based Storage* **Moses Tade**, Curtin University				
12:00 – 12:30	*All Wastes are not Equal for Hydrogen Production via Gasification* **Josephine Mary Hill**, University of Calgary				
12:30 - 13:30	**Lunch**				
	Distinguished Speakers Session 8 **Venue**: *Saqr Ballroom* **Chairs**: Fengqi You, Zachary W. Ulissi				
13:30 – 14:00	*Flame Aerosol Synthesis of High-Entropy Catalysts for Sustainability* **Mark T. Swihart**, University at Buffalo				
14:00 – 14:30	*Engineering Human+AI Collaboration for Process Safety and Sustainability Applications* **Rajagopalan Srinivasan**, Indian Institute of Technology Madras				
14:30 – 15:00	*Artificial Intelligence for Multiphase Reactors: Some Recent Advances* **Muthanna H. Al-Dahhan**, Missouri University of Science & Technology				
15:00 - 15:30	**Coffee Break and Poster Session 3**				
	Distinguished Speakers Session 9 **Venue**: *Saqr Ballroom* **Chairs**: Sossina M. Haile, Bhavik Bakshi				
15:30 – 16:00	*Computational Screening of Metallic and Mixed-metal Oxide Catalysts for Bio-oils Upgrading and H_2 Production* **Lourdes Vega**, Khalifa University				
16:00 – 16:30	*Outlook on Global Energy Transition: AI Catalysing Power Sector Transformation* **Gauri Singh**, International Renewable Energy Agency				
16:30 – 17:00	*Revisiting Energy Systems Modelling in the Context of AI* **Rangan Banerjee**, Indian Institute of Technology Delhi				
17:00 - 17:30	**Closing Remarks and Award Ceremony**				
17:30 – 19:00	Visit to the Sheikh Zayed Grand Mosque				

TECHNICAL PROGRAM (Parallel Sessions 1 – 3)

Monday, 15th December 2025			
Session	**Parallel Session 1** ***AI for Sustainable Chemical Processes***	**Parallel Session 2** ***Process Intensification for Sustainability***	**Parallel Session 3** ***Sustainable Materials for Energy Storage***
Room	Saqr Ballroom 1	Saqr Ballroom 2	Saqr Ballroom 3
Chairs	**Suprakas Sinha Ray** **Shelaka Gupta**	**Manoj Ramteke** **Ejaz Ahmed**	**Madhulika Gupta** **Rajesh Kumar Upadhyay**
16:00 – 16:20	*Generative AI for Sustainability: Applications in Drug Discovery, Agrichemistry and Materials Science* **Alex Aliper** Insilico Medicine	*Sustainable Nanocomposites Synthesized through "Green" Plasma Induced Liquid Chemistry* **Dan Sun** Queen's University Belfast	*Hybrid Materials as Electrode and Electrolyte for Conversion Devices* **Suddhasatwa Basu** IIT Delhi
16:20 – 16:40	*Accelerating Sustainable Technologies through High-Throughput Synthesis of Covalent Organic Frameworks* **Safiya Khalil Al Hashmi** NYU Abu Dhabi	*Catalytic Structures for CO_2 Conversion into Lower Hydrocarbons: Structure-Resolved CFD Simulations* **Vivek Buwa** IIT Delhi	*Atomic Scale Origin of RC-Circuit Behavior in Solid Electrolytes* **Abhijit Chatterjee** IIT Bombay
16:40 – 17:00	*Making Artificial Intelligence Work in the Molecular Sciences* **Johannes Hachmann** University at Buffalo	*Next-Generation Anion Exchange Membranes with Superior Stability and Conductivity for Electrochemical Energy and Water Electrolysis* **Bijay Tripathi** IIT Delhi	*Catalytic Layered Double Perovskites for Sustainable Fuel Cells and Electrolyzers* **Sivaprakash Sengodan** Khalifa University
17:00 – 17:20	*Enhanced Sampling Augmented with Machine Learning Methods for Simulating Activated Processes* **Tarak Karmakar** IIT Delhi	*Ion Transport in Electrochemical Capacitors: Modified Kirchhoff's Law for Structure-Property Relationships* **Ankur Gupta** University of Colorado	*Extraction of Vanadium from Spent Catalyst and Utilization in Flow Battery* **Anil Verma** IIT Delhi
17:20 – 17:40	*Machine Learning Based Dynamic Model of Solar Thermal Power Plant* **Mani Bhushan** IIT Bombay	*Intelligent Digital Twins - Transforming the Energy Industry* **Sriganesh Karur** Ex-General Manager, Shell	*New Materials for Clean Energy and Sustainability* **Ahsan Qurashi** Khalifa University

TECHNICAL PROGRAM (Parallel Sessions 4 – 6)

Tuesday, 16th December 2025			
Session	**Parallel Session 4** ***Materials for Sustainability I***	**Parallel Session 5** ***Carbon Capture & Beyond***	**Parallel Session 6** ***AI for Sustainability I***
Room	Saqr Ballroom 1	Saqr Ballroom 2	Saqr Ballroom 3
Chairs	**Deepak Kumar** **Suddhasatwa Basu**	**Husain Kanchwala** **Ramakrishna R Sonde**	**Abhijit Chatterjee** **Sriganesh Karur**
15:30 – 15:50	*Computational Modeling and ML to Discover Materials and Reaction Pathways for Clean Energy Applications* **Ananth Govind Rajan** IISc Bangalore	*High-throughput Molecular and Process-level Screening of COFs for Carbon Capture via Pressure Swing Adsorption* **Ashutosh Yadav** IIT Jammu	*Engineering Polymer-surface Adhesion using Molecular Dynamics and Machine Learning* **Divya Nayar** IIT Delhi
15:50 – 16:10	*Zeolite-templated Carbon-based Air Electrodes for Lithium-Oxygen Battery* **Maryam Khaleel** Khalifa University	*Developing Nanostructured Catalysts for CO_2 Conversion using Density Functional Theory and Machine Learning* **Sergey Kozlov** NUS, Singapore	*Optimizing Renewable Energy and Thermal Storage with Advanced AI* **Martin Takáč** MBZUAI, Abu Dhabi
16:10 – 16:30	*Rational Design of Acidic Sites for Large Pore Zeolite for their Effective Utilization in Alkylation Reactions for Sustainable Aviation Fuel* **Manjesh Kumar** IIT Delhi	*Phonon Pathways to Green Energy: Thermoelectric Advances in 2D Chalcogenides* **Nirpendra Singh** Khalifa University	*Artificial Intelligence-Driven Optimization of Solid Oxide Electrolysis for Efficient Green Hydrogen Production* **Munawar A. Shaikh** UAE University
16:30 – 16:50	*Tunable Frameworks: Fit-to-Purpose Materials for Energy and Sustainability* **Dinesh Shetty** Khalifa University	*A Novel Carbon Capture and Utilization Technology to Recycle Heavy Metals from Industrial Waste* **Vikram Singh** IIT Delhi	*Development of Deep Learning based Bayesian Sensor Fusion Algorithms: Application to Hybrid Three Tank Experimental System* **Jayaram Valluru** IIT Ropar
16:50 – 17:10	*Bioplastics in Focus: Life Cycle Assessment and AI for a Greener Future* **Suprakas Sinha Ray** DSI - CSIR	*Computational-Guided Design of Functionalized Zeolite-Templated Carbons for Efficient CO_2 Capture* **Daniel Bahamon Garcia** Khalifa University	*Mapping the Elastic Properties of Sodium Silicate Glasses: A Simulation Pipeline Integrating SHIK and DeepMD with XGBoost for High-Fidelity Prediction* **Hicham Jabraoui,** TII
17:10 – 17:30	*Data-Driven Materials Designing for Optoelectronics* **Dibyajyoti Ghosh** IIT Delhi	*Climate Change, Sustainability and the Pathway Towards a Circular Economy: Global Perspectives and Challenges* **Chithirai Pon Selvan** Curtin University Dubai	*Machine Unlearning for Process Applications* **Manoj Ramteke** IIT Delhi

TECHNICAL PROGRAM (Parallel Sessions 7 – 9)

Wednesday, 17th December 2025			
Session	**Parallel Session 7** ***Sustainable Chemical Processes***	**Parallel Session 8** ***AI for Sustainability II***	**Parallel Session 9** ***Materials for Sustainability II***
Room	Saqr Ballroom 1	Saqr Ballroom 2	Saqr Ballroom 3
Chairs	**Mani Bhushan** **Munawar A. Shaikh**	**Dinesh Shetty** **Ashutosh Yadav**	**Anil Verma** **Dibyajyoti Ghosh**
08:00 – 08:20	*Direct Joule-Heated Membrane Reformer for On-Site Production of Ultra-pure Hydrogen* **Rajesh Kumar Upadhyay** IIT (BHU) Varanasi	*Artificial Intelligence – Driven Screening and Atomistic Simulation of Corrosion Inhibitors for Steel in Marine Environments* **Shivraj Karewar** Technology Innovation Institute	*Porous Organic and Coordination Polymer Materials for Energy and Environment Sustainability* **Himanshu Aggarwal** BITS Pilani, Hyderabad
08:20–08:40	*Adsorption of Two Anionic Mordant Red Dyes by Differently Activated Plant Derived Biochar* **Umesh Mishra** NIT Agartala	*Prediction of Descriptor (CO and OH) Binding Energy on Cu-based Bimetallic Alloys using ML Approach* **Shelaka Gupta** IIT Hyderabad	*Microwave-Synthesized Graphene Quantum Dots as Hydrophilic Modifiers for High-Performance Polysulfone Ultrafiltration Membrane* **Jagdeeshbabu P Ettiyappan** NITK Surathkal
08:40-09:00	*Magnesium-CaNi Composite Systems for Hydrogen Storage Applications* **Nitesh Kumar** IIT Jammu	*Graph Neural Network Assisted Sensor Placement Design using Reliability Criteria* **Om Prakash** IIT Delhi	*Microarchitected Hierarchically Porous PLA/S/CNT Nano-composite Electrodes Enabled via 3D Printing with Remarkable Performance in Li-Ion Batteries* **Vinay Gupta** Khalifa University
09:00-09:20	*Deciphering the Role of Metals and Promoter Loading on CO_x Free Turquoise H_2 Production for Carbon Neutral Coal Mining* **Ejaz Ahmad** IIT (ISM) Dhanbad	*Deconstruction of Biomass for Bioenergy: Molecular Insights into Xylan-Cellulose Adhesion* **Madhulika Gupta** IIT (ISM) Dhanbad	*Core-shell Nanotechnology Assisted Nano-Composite Anode (Gr/Si@TiO_2) for Li-ion Battery* **Deepak Kumar** IIT Delhi
09:20-09:40	*Radiation-based Techniques for Detailed Investigation of Cohesive Particle Flows to Make Advanced Materials* **Ruud van Ommen** Delft University of Technology	*Tuning the Selectivity of Hydrogenation and C-C Coupling Pathways during Biomass Conversion* **Rachit Khare** Technical University of Munich	*Graphene Anti-Corrosion Coatings for Sustainable Infrastructure and Industrial Efficiency* **Husain Kanchwala** IIT Delhi

TECHNICAL PROGRAM
(Young Researchers and Scientists Sessions)

Monday, 15th December 2025	
Session	**YRS Session 1** ***AI & ML for Sustainability***
Room	Al Reem, Fairmont Bab Al Bahr, Abu Dhabi
Chairs	**Jayaram Valluru, Divya Nayar**
16:00 – 16:10	*Metal Chalcogenide Nanomaterials for Sustainable Development*, **Shivram Garje,** University of Mumbai
16:10 – 16:20	*AI-Guided Screening of 2D-Materials for Efficient Proton Transport in PEM Fuel Cells,* **Yuting Li**, Khalifa University
16:20 – 16:30	*Development of a Multifunctional Cellulose/Chitosan Bioelectrode for Neural Interfacing Applications using Machine Learning Approaches,* **Meera Alex,** American University of Sharjah
16:30 – 16:40	*Mapping the Flammability Space of Sustainable Refrigerant Mixtures through an Artificial Neural Network Based on Molecular Descriptors,* **Sultan Al Ali**, Khalifa University
16:40 – 16:50	*DOS is More: Physics-Informed GNNs for Sustainable Materials*, **Elizaveta Starykh**, MBZUAI
16:50 – 17:00	*A Hyper-Heuristic Interval based AI Prediction Model for Reliable Performance Forecasting of Water Energy Nexus System*, **Bukke Kiran Naik**, NIT Rourkela
17:00 – 17:10	*Zeolite – Conducting Polymer Nanocomposite for Water Remediation Coupled with Machine Learning Insights*, **Megha Parmar**, Pandit Deendayal Energy University
17:10 – 17:20	*Hourly Solar Irradiation Forecasting via Hybrid Facebook Prophet-ML Framework for Amravati* Region, **Aditya Kumar**
17:20 – 17:30	*Data-Driven Machine Learning Applications for Predictive Modeling of Petrochemical and Ecofriendly Systems*, **Noora Al Mansoori**, Abu Dhabi University
17:30 – 17:40	*Prompt Learning Framework for Zero-Shot Carbon Fiber Defect Detection in Hydrogen Storage Manufacturing*, **Samee Ullah Khan**, Khalifa University

TECHNICAL PROGRAM
(Young Researchers and Scientists Sessions)

Tuesday, 16th December 2025	
Session	**YRS Session 2** ***Materials for Sustainability***
Room	Al Reem, Fairmont Bab Al Bahr, Abu Dhabi
Chairs	**Tarak Karmakar, Bijay Tripathi**
15:30 – 15:40	*Microwave-Assisted Synthesis of $ZnFe_2O_4$ Nanomaterials for High-Performance Supercapacitor Application*, **Pavan Dhurandhar**, University of Mumbai
15:40 – 15:50	*Engineering Sustainable Materials and Methods for Lightweight Lattice Structures*, **Asha Viswanath**, Khalifa University
15:50 – 16:00	*Export Competitiveness of Controlled Environment Saffron Production: Entrepreneurial Evidence from Indian Emerging States*, **Sahiba Sharma,** Manav Rachna University, Faridabad
16:00 – 16:10	*Morphological Engineering of $CoFe_2O_4$ Nanostructures for High-Performance and Durable Supercapacitor Electrodes*, **Rukayat Zakari**, Khalifa University
16:10 – 16:20	*From Nature to Power: Eco-Friendly Energy Scavenging and Self-powered Smart Sensing*, **Bushara Fatma**, Khalifa University
16:20 – 16:30	*Advanced Inorganic Materials for Energy Storage Devices*, **Rohan Narkar**, University Of Mumbai
16:30 – 16:40	*Electromagnetic Shielding Performance of Large Lateral-Sized Graphene Sheets* **Shanavas Shajahan**, Khalifa University

TECHNICAL PROGRAM
(Young Researchers and Scientists Sessions)

Wednesday, 17th December 2025	
Session	**YRS Session 3** ***Catalysis and Carbon Capture***
Room	Al Reem, Fairmont Bab Al Bahr, Abu Dhabi
Chairs	**Ananth Govind Rajan, Manjesh Kumar**
08:00 – 08:10	*Selective Formation of Formic Acid via Low-Temperature Methane Oxidation on Au-Fe/Na-ZSM-5: Experimental and DFT Insights*, **Iqra Ahangar**, Higher Colleges of Technology, Abu Dhabi
08:10 – 08:20	*Ni-Ru Catalysts for Biogas Reforming: Mitigating Carbon and Sulfur Induced Deactivation via MoO_3 Promotion*, **Satyajit Panda**, Council of Scientific & Industrial Research, Dehradun
08:20 – 08:30	*Facile Hydrothermal Synthesis of MoS_2/MXene Composite for Efficient Rhodamine B Dye Adsorption from Aqueous Solutions*, **Riddhi Patel**, Pandit Deendayal Energy University, Gandhinagar
08:30 – 08:40	*Synthesis-dependent function of Pd/CHA Zeolites under Cold-start conditions: An Operando FT-IR Spectroscopy and Microreactor Study*, **Yusra Hamid**, University of Lisbon
08:40 – 08:50	*Nonpolynomial Spline Approach for CO_2 Adsorption–Diffusion Modelling*, **Kirandeep Kaur**, Netaji Subhash University of Technology Delhi
08:50 – 09:00	*Integrated Experimental, Simulation, and Process-level Evaluation of Advanced Adsorbents for PSA-based CO_2 Capture in Cement Plants*, **Khushboo Yadava**, Grihitum, IIT Mandi Catalyst
09:00 – 09:10	*Photocatalytic Degradation of Sulfamethoxazole with TiO_2-Fe_2O_3 Photocatalyst under Solar Light Irradiation*, **Jitendra Pal Salavadhi**, NITK, Surathkal
09:10 – 09:20	*Conformational Dynamics of O-2 Acetylated Xylan on Cellulose Surfaces: Implications for Sustainable Biofuel Production*, **Tripti Kundu**, IIT (ISM) Dhanbad
09:20 – 09:30	*Barriers for Integrating Carbon Capture and Storage into Net-Zero Pathways: A Comprehensive Literature Review*, **Priji Biju**, The British University in Dubai

TECHNICAL PROGRAM
(Young Researchers and Scientists Sessions)

Wednesday, 17th December 2025	
Session	**YRS Session 4** ***Water-Energy-Climate***
Room	Sir Banyas, Fairmont Bab Al Bahr, Abu Dhabi
Chairs	**Vikram Singh, Ankur Gupta**
08:00 – 08:10	*Sustainable Extraction of Rare Earth Element: Repurposing Waste Fungal Pellets for Lanthanum (La) Recovery from Wastewater*, **Bharat Bhushan**, IIT Guwahati
08:10 – 08:20	*Enhancing Water Droplet Erosion Resistance through in-situ Austenite-to-Martensite Phase Hardening*, **Lama Mahmoud**, Concordia University
08:20 – 08:30	*Development of Low-Carbon Thermoplastic Pellets for Additive Manufacturing*, **Reem Al Ramsi**, Technology Innovation Institute, Abu Dhabi
08:30 – 08:40	*Revolutionary Holey Graphene-hydrophobic Eutectic Solvent-embedded Sulfonated PES Hybrid Membranes for Superior Emerging Contaminant Removal*, **Anjali Singhal Goyal**, Khalifa University
08:40 – 08:50	*Porous rGO/networked Cellulose Composite Membranes: Towards Enhanced Nanofiltration Performance of rGO-based Membranes*, **Shabin Mohammed**, Higher Colleges of Technology, Abu Dhabi
08:50 – 09:00	*A Sustainable Hybrid Chemical-bioflocculant (HCBF) for the Removal of Polystyrene Microplastics from Water Treatment Plants*, **Priya Krishnamoorthy Lekshmi Ammal**, TKM College of Engineering
09:00 – 09:10	*Performance Enhancement of Type IV Hydrogen Tanks Using Expanded Graphite*, **Omar El Khatib**, Khalifa University

TECHNICAL PROGRAM
(Lightning Sessions)

Monday, 15th December 2025	
Session	**Lightning Session 1**
Room	Sir Banyas, Fairmont Bab Al Bahr, Abu Dhabi
Chairs	**Om Prakash, Rachit Khare**
16:00	*Deep Neural Network–Based Dynamic Plantwide Modeling of a Hybrid Solar Thermal Power Plant*, **Dibyajyoti Baidya**, IIT Bombay
16:05	*Machine Learning-Driven TMDCs-based Sensors for Discrimination of Volatile Amines in Complex Mixtures*, **Snehraj Gaur**, IIT Delhi
16:10	*Development of Machine Learning Integrated Moving Horizon State Estimator for Processes Subject to Missing Data and Delayed Measurements: Application to Industrial Scale Penicillin Production Process (IndPenSim)*, **Vishnu Roshan**, IIT Ropar
16:15	*Optimizing Sustainable Energy Planning in Delhi: A Hybrid Machine Learning and Time Series Approach for Solar Potential Forecasting*, **Dipali Pawar**, IIT Delhi
16:20	*Sound Absorption Prediction in TPMS Metamaterials via Machine Learning*, **Vignesh Sekar**, Khalifa University
16:25	*AI-ML Aided Advanced Technologies For Maintenance and Sustainability of Civil Infrastructure: Field Study On Real Rail over Bridge*, **Shipra Prakash**, IIT Delhi
16:30	*AI-Driven Wind Resource Modeling for Efficient Wind-to-Hydrogen System Design at Jaisalmer*, **Nagasree Keerthi Pujari**, IIT Hyderabad
16:35	*Explainable Machine Learning Based Multi-Objective Optimization Framework for Ammonia Recovery from Digestate*, **Shobhita Sharma**, IIT Delhi
16:40	*Machine Learning Potentials to Guide Reaction Mechanisms at the Metal-Water Interface*, **Jayendran Iyer**, IIT Delhi
16:45	*MAX Phase Purity–Dependent Interlayer Spacing Engineered Ti_3C_2-F MXene Electrodes for High-performance Energy Storage Applications*, **Ekta Choudhary**, IIT Indore
16:50	*Artificial Intelligence Driven Forecasting of Solar-Based Green Hydrogen Production for Sustainable Energy Development in India*, **Karan Sareen**, IIT Delhi/CEA
16:55	*Boosting Hydrogen Evolution on Halogenated MXenes via Surface Termination Engineering: A Data-Informed Computational and Experimental Strategy*, **Ankita Kumari**, IIT Delhi
17:00	*Data-Driven Prediction of Polymer Adhesion on Heterogeneous Surfaces via Attention Based Learning*, **Sibasankar Panigrahy**, IIT Delhi
17:05	*Production of H_2-rich Syngas Production through ML-driven Catalyst and Process Condition Optimization with Experimental Validation and Mechanistic Insights*, **Kaushik Kundu**, IIT Delhi
17:10	*A Context-Dependent Network DEA Framework with Directional Distance Functions for Sustainable Decision Intelligence: Insights from the Indian Banking Sector*, **Akash Jain**, NSUT Delhi
17:15	*Unveiling Chemical Evolution of Electrode-electrolyte Interface in Sodium Ion Batteries from Machine Learning Potential-based Simulations*, **Dhananjay**, IIT Delhi

TECHNICAL PROGRAM
(Lightning Sessions)

Tuesday, 16th December 2025	
Session	**Lightning Session 2**
Room	Sir Banyas, Fairmont Bab Al Bahr, Abu Dhabi
Chairs	**Joby Joseph, Nidhi Jain**
15:30	*Hydrogen Storage Capacities in Nanoporous M2(m-dobdc) Metal-Organic Frameworks at Near Ambient Temperatures*, **Himani Joshi**, IIT Indore
15:35	*From Bulk Solvents to Confined Spaces: Redefining Reaction Environments*, **Mohd Ussama**, IIT Delhi – Abu Dhabi
15:40	*Photonics to Physiology: BCN@CMC Nanocomposites for Optoelectronics and Biomedical Devices*, **Mohan Manjunathaswamy**, Khalifa University
15:45	*Unveiling Medium-Dependent Synergistic Role of Metals and Active sites in Prussian Blue Analogue-Derived FeCoTe for Hydrogen Evolution using Electroanalytical Techniques*, **Bhawna Rathor**, IIT Delhi
15:50	*Novel Tri-Amine Blend for Efficient Post-Combustion CO_2 Capture: Experimental Absorption–Desorption Studies, Kinetic Analysis, Modeling, and Spectroscopic Investigations*, **Akhil Kumar Gupta**, IIT (BHU) Varanasi
15:55	*Investigating the Electrochemical Performance and Degradation Mechanism of $Na_3V_2(PO_4)_3$ for Sodium-Ion Batteries*, **Akshita Sharma**, IIT Delhi
16:00	*An Integrated Process-Structure-Property Model for Recycled Carbon Fibre Needle Punched Nonwovens: Towards Sustainable Structural Materials*, **Danvendra Singh**, IIT Delhi
16:05	*Surface-Engineered Pd/g-C_3N_4 Catalysts for Light-Driven Formic Acid Dehydrogenation at Room Temperature*, **Mathivathani J R**, IIT Delhi
16:10	*Eco-friendly Co-precipitation Processed $BaZn(VO_4)_2$ Nanoparticles as a Promising Anode Material for Li and Na-ion Batteries*, **Mohd Saqib**, IIT Delhi
16:15	*Green Encapsulation of Metal Oxide and Noble Metal ZnO@Ag for Efficient Antibacterial and Catalytic Performance*, **Aisha Noor**, IIT Delhi
16:20	*Synthesis of Butyl Butyrate as a Sustainable Aviation Fuel Using V_2O_5-Supported Silicomolybdic Acid Catalyst*, **Shariq Farhan Elahi**, Curtin University, Australia and IIT (ISM) Dhanbad, India
16:25	*Interfacial Charge Transfer Dynamics in Electrochemical CO_2 Reduction on Gold Electrodes: Influence of Ionic Strength and Cation Identity in Na_2CO_3-Based Electrolytes*, **Jagriti Malik**, IIT Delhi
16:30	*Biomass Briquettes as a Low-Carbon Alternative Fuel for Hard-to-Abate Industries*, **Bishakh Choudhury**, IIT Delhi
16:35	*Exploring MOF – Hydrocarbon Integration for Sustainable Adsorption Cooling: An Accelerated Approach using Bayesian Optimization and Monte Carlo Simulations*, **S Muthukrishnan**, IIT Kanpur
16:40	*High-κ Interface Engineering for Energy-Efficient Spin–Orbit Torque Memories: A Materials Pathway Toward Digital Sustainability*, **Shubham Bhatt**, IIT Delhi
16:45	*Unexpected Lowering of Charge-Transfer Resistance in Ultra-Long Cycled (>30,000 Cycles) Solution-Processed Laminar-Crystalline Li_3VO_4 Anodes and its Li_3VO_4||LFP Full Cells Performance in 18650 form factor*, **Tejveer Singh Anand**, IIT Delhi
16:50	*Techno-Economic Analysis of Green Hydrogen Project in Abu Dhabi*, **Adnan Nagah**, Abu Dhabi National Oil Company (ADNOC) and IIT Delhi – Abu Dhabi

Poster Sessions

TECHNICAL PROGRAM (Poster Sessions)

Monday, 15th December 2025	
Session	**Poster Session 1**
Room	Lobby, Fairmont Bab Al Bahr, Abu Dhabi
Poster No.	**Title**
P1-01	*Optimizing Dendrite Free Anodes for Zinc Ion Batteries using PEG functionalized Carbon Nanotube*, **Abdullah Shaikh**, Khalifa University
P1-02	*Finding a Best Catalysis for a Plasma Based Ammonia Synthesis with the Help of Agglomeration Energy by DFT*, **Aneesh Kumar S**, IIT Delhi – Abu Dhabi
P1-03	*Hydrophobic Deep Eutectic Solvent–Embedded Ultrafiltration Membranes for Efficient Pharmaceuticals Removal from Municipal Wastewater*, **Anjali Goyal**, Khalifa University
P1-04	*Optimizing Ferroelectric Photovoltaic Performance in KBNNO Ceramics via Grain Size Engineering*, **Ankit Chahar**, Jawaharlal Nehru University New Delhi
P1-05	*Investigating Thermal Performance of PCM-Based Thermal Energy Storage with Porous Fins: A Coupled CFD - ML Approach*, **Ankit Kumar**, IIT Delhi – Abu Dhabi
P1-06	*Machine Learning Approaches for Prediction of the Coefficient of Discharge of Broad Crested Weirs*, **Ashwin Chitravanshi**, IIT (BHU) Varanasi
P1-07	*Sustainable Oil Spill Cleanup Using Milkweed–Waste Cotton Needle-Punched Nonwoven Blends*, **Chandra Jeet Singh**, IIT Delhi
P1-08	*Materials-Led Passive Cooling Retrofit for a Lecture Hall in Abu Dhabi*, **Deepanshu Babbar**, IIT Delhi – Abu Dhabi
P1-09	*Circular Valorization of Textile Wastewater in Concrete Production: A Sustainable Material Approach for Water–Energy Nexus*, **Deepti Surana**, IIT Delhi
P1-10	*Designing Heat-Resistant Self-Healable Adhesives through Polybenzoxazine Vitrimers with Dual Dynamic Networks*, **Gaurav Rai**, IIT Delhi
P1-11	*Pyrolysis of Electrostatically Enriched Precursors Produce Pt_3Ni Nanocatalysts Supported on Nitrogen-doped GO with a Low Overpotential for HER* , **Hafna T**, IIT Palakkad
P1-12	*Nanostructured Polybenzoxazine Particles-Supported Ammonia Borane for Hydrogen Storage and Release*, **Ingita Tiwari**, IIT Delhi
P1-13	*Machine Learning Based Dynamic Model of Solar Thermal Power Plant*, **Mani Bhushan**, IIT Bombay
P1-14	*Harnessing Mechanical Energy with Rotationally Aligned Piezoelectric TMDs Composite Materials: A Step Toward Flexible and Sustainable Energy Storage Systems*, **Mayuri Srivastava**, IIT Delhi
P1-15	*Interface-Engineered Polyaniline Composites on Diverse Supports for Efficient Michael Addition Catalysis*, **Md Imteyaz Alam**, IIT Delhi
P1-16	*Development of Sulphur and Nitrogen Doped Fluorescent Carbon Quantum Dots for Hydroquinone Sensing*, **Murli Dhar Mitra**, IIT (BHU) Varanasi
P1-17	*Development of a Correlation for Assessment of BIPV Potential Under Shading Constraints*, **Priyanka Rai**, Malaviya National Institute of Technology Jaipur
P1-18	*Low Temperature Oxidation of Ethylene by Co_3O_4 Catalysts* , **Roshni Madampadi**, IIT Palakkad
P1-19	*Hybrid Conductive Additive for Stable Graphite-Based Li-ion Anodes*, **Rudraksh Gupta**, IIT Delhi

TECHNICAL PROGRAM (Poster Sessions)

Monday, 15th December 2025	
Session	**Poster Session 1**
Room	Lobby, Fairmont Bab Al Bahr, Abu Dhabi
Poster No.	**Title**
P1-20	*Cadmium Ion Removal from Wastewater using Activated Carbon under Variable Experimental Condition*, **Shahid Ikabal**, IIT (ISM) Dhanbad
P1-21	*Analyzing Charging Performance of High Temperature Shell and Tube Latent Heat Storage*, **Mallayya Swami**, IIT Delhi
P1-22	*Hourly Ahead Solar Irradiation Forecasting using Deep Learning Models*, **Tarun Goel**, IIT Delhi
P1-23	*Eco-inspired Multifunctional Hydrogels via Free-Radical Polymerization for Ultra-Sensitive Sensing, Recovery, and Reuse of Rare Earth Elements*, **Somya Sadaf**, IIT Gandhinagar
P1-24	*Wastewater to Wardrobe: Phycocyanin from Oxygenic Photogranules for Eco-Functional Textiles*, **Vivek Kumar Nair**, IIT Delhi
P1-25	*Synergistic g-C_3N_4/$BiFeO_3$ Binder-free Cathode: Sustainable Photoelectron Oxidation of Dimethyl Phthalate*, **Yasser Bashir**, IIT Delhi
P1-26	*Understanding Pd/CHA Zeolites Function under Cold-Start Conditions: An Operando FT-IR Spectroscopy and Microreactor Approach*, **Yusra Hamid**, University of Lisbon
P1-27	*Reusing End-of-Life Solar PV Panels as Silicon Anodes for Lithium-Ion Batteries: A Review*, **Zarrin Khan**, IIT Bombay
P1-28	*Life Cycle Assessment of Methane Abatement Technologies using Small Language Model Mixture of Experts*, **Bilal Rasheed**, IIT Delhi – Abu Dhabi
P1-29	*Climate-Justified Optimization for Decentralized Ammonia Production via Green Hydrogen and Haber-Bosch Process using Deep Learning*, **Mehbooba C**, IIT Delhi – Abu Dhabi
P1-30	*Multi-Objective Superstructure Optimization and Techno-Economic Assessment of Electrified CO_2 to Methanol Conversion*, **Sarthak Mazumder**, IIT Delhi – Abu Dhabi
P1-31	*Integrating Science, Engineering, and Policy for Sustainable Aerospace Innovation in Africa*, **Yasir Aliyu**, UAVS
P1-32	*Machine Learning Enhanced Prediction of Voltage Capacity Dynamics in Gradient Aged Lithium-Ion Batteries*, **Jibin M Joy**, IIT Delhi – Abu Dhabi
P1-33	*Optimizing Land and Energy: Sustainable Underground Storage for a Resilient Energy Transition*, **Altaf Usmani**, Engineers India Limited
P1-34	*Bimetallic $CoCdS_2$: A Promising Supercapacitor Material for Energy Storage Devices*, **Pratiksha Borse**, University of Mumbai
P1-35	*Production of CO_2 Adsorption on Data-Driven Metal Organic Frameworks (MOFs) using Machine Learning*, **Ashutosh Yadav**, IIT Jammu
P1-36	*Machine-Learned Solvent-Implicit Coarse-Grained Modeling of Biomimetic Lipid Bilayers*, **Ayishwarya Dutta**, IIT Delhi – Abu Dhabi
P1-37	*Liquid Structure of Localized High Concentration Electrolyte for Lithium-Ion Battery*, **Navneet Singh**, IIT Delhi – Abu Dhabi
P1-38	*Design of Material (Metal Organic Framework) for Carbon Capture: A Computational Approach Integrated with Atomistic Simulation*, **Tanay Das**, IIT Delhi - Abu Dhabi

TECHNICAL PROGRAM (Poster Sessions)

Tuesday, 16th December 2025	
Session	**Poster Session 2**
Room	Lobby, Fairmont Bab Al Bahr, Abu Dhabi
Poster No.	**Title**
P2-01	*Wind Power Forecasting Using Various Forecasting Techniques*, **Aditya Kumar**, NIT Trichy
P2-02	*Smart Multi-Layered Wall Insulation Using Recycled Waste Materials*, **Ahmad Deeb**, Khalifa University
P2-03	*A Context-Dependent Network DEA Framework with Directional Distance Functions for Sustainable Decision Intelligence: Insights from the Indian Banking Sector*, **Akash Jain**, Netaji Subash University of Technology Delhi
P2-04	*Impact of Dual Acetylation and Temperature on Xylan-Cellulose Interactions*, **Ankit Joshi**, IIT (ISM) Dhanbad
P2-05	*Boosting Hydrogen Evolution on Halogenated MXenes via Surface Termination Engineering: A Data-Informed Computational and Experimental Strategy*, **Ankita Kumari**, IIT Delhi
P2-06	*Sound Absorption Prediction in TPMS Metamaterials via Machine Learning*, **Vignesh Sekar**, Khalifa University
P2-07	*Hybrid-CGAN-Based Modeling and Experimental Study of Thermal Comfort in Extreme Mining Protective Clothing*, **Bukke Kiran Naik**, NIT Rourkela
P2-08	*Deep Neural Network–Based Dynamic Plantwide Modeling of a Hybrid Solar Thermal Power Plant*, **Dibyajyoti Baidya**, IIT Bombay
P2-09	*Optimizing Sustainable Energy Planning in Delhi: A Hybrid Machine Learning and Time Series Approach for Solar Potential Forecasting*, **Dipali Pawar**, IIT Delhi
P2-10	*Carbide Volume Fraction in Cobalt-based Alloys using ML techniques*, **Vishakh Pradeep Kumar**, Heriot-Watt University
P2-11	*Development of Multifunctional Textiles using Bio-derived Coumalic Acid against Pathogens, Vector-borne Diseases, and Environmental Stressors*, **Gulshitab Aalam**, IIT Delhi
P2-12	*Development of Machine Learning Integrated Moving Horizon State Estimator for Processes Subject to Missing Data and Delayed Measurements: Application to Industrial Scale Penicillin Production Process (IndPenSim)*, **Vishnu Roshan**, IIT Ropar
P2-13	*Machine Learning Potentials to Guide Reaction Mechanisms at the Metal-Water Interface*, **Jayendran Iyer**, IIT Delhi
P2-14	*Bioinspired Metamaterials for Sustainable Noise Reduction*, **Kamal K Sirivuri**, Khalifa University
P2-15	*Production of H_2-rich Syngas Production through ML-driven Catalyst and Process Condition Optimization with Experimental Validation and Mechanistic Insights*, **Kaushik Kundu**, IIT Delhi
P2-16	*Forecasting Building Thermal Demand Using Machine Learning*, **Lloyd Corcoran**, Cardiff University
P2-17	*AI-Driven Local Positioning System for Secure and Autonomous Navigation in Resource-Constrained Environments*, **Misgina Tewelde**
P2-18	*CNN-LSTM Based Multi-Height Wind Speed Prediction for Sustainable Wind Energy Applications*, **Mohan Narayan Gupta**, IIT (BHU) Varanasi
P2-19	*Data-Driven Catalytic Depolymerization of Lignin: Sobol–Bayesian Optimization Framework for High-Yield Guaiacol Production*, **Nagasree Keerthi Pujari**, IIT Hyderabad

TECHNICAL PROGRAM (Poster Sessions)

Tuesday, 16th December 2025	
Session	**Poster Session 2**
Room	Lobby, Fairmont Bab Al Bahr, Abu Dhabi
Poster No.	**Title**
P2-20	*High-Throughput and Data-Driven Search for Stable Optoelectronic $AMSe_3$ Materials*, **Nikhil Singh**, IIT Delhi
P2-21	*Data-Driven Indoor Air Quality Forecasting: A Machine Learning Approach for Smart and Healthy Buildings*, **Sajid Mannan**, IIT Delhi
P2-22	*Industrial-Scale Prediction of Cement Clinker Phases using Machine Learning*, **Sheikh Junaid Fayaz**, IIT Delhi
P2-23	*Explainable Machine Learning Based Multi-Objective Optimization Framework for Ammonia Recovery from Digestate*, **Shobhita Sharma**, IIT Delhi
P2-24	*Data-Driven Prediction of Polymer Adhesion on Heterogeneous Surfaces via Attention based Learning*, **Sibasankar Panigrahy**, IIT Delhi
P2-25	*Machine Learning-Driven TMDCs-based Sensors for Discrimination of Volatile Amines in Complex Mixtures*, **Snehraj Gaur**, IIT Delhi
P2-26	*AI-Enabled Design Verification and Validation: Strengthening Process Safety through Intelligent Engineering Assurance*, **Subhadra Devi Saripalli**, IIT Madras
P2-27	*Artificial Neural Network Framework for Exploring the Flammability Space of Eco-Friendly Refrigerants*, **Sultan Al Ali**, Khalifa University
P2-28	*Basal Plane Passivation of $Ti_3C_2T_x$ MXenes through Prussian Blue Analog Nanoparticles Anchoring for Efficient and Selective Electrochemical Ammonia Synthesis*, **Aamir Yaseen Bhat**, IIT Delhi
P2-29	*Boosting Mg Battery Performance using InSe/C Composite Cathode*, **Gazal Gupta**, IIT Delhi
P2-30	*Suppressing Agglomeration and Boosting Proton Storage in 1D Mesoporous Co_3S_4-Carbon Nanofiber Composites for Flexible Supercapacitors*, **Sagar Munjal**, IIT Delhi
P2-31	*Experimental Investigation of Charging and Discharging Pattern of a Shell and Tube Thermal Energy Storage System*, **Sudhir Kumar Gupta**, IIT Delhi
P2-32	*Comprehensive Life Cycle Assessment of CO_2-Enhanced Oil Recovery Pathways in Indian Oilfields: Evaluating Emission Trade-offs and Net Carbon Balance*, **Dinesh Joshi**, Khalifa University
P2-33	*Unexpected Lowering of Charge-Transfer Resistance in Ultra-Long Cycled (>30,000 Cycles) Solution-Processed Laminar-Crystalline Li_3VO_4 Anodes and its Li_3VO_4||LFP Full Cells Performance in 18650 form factor*, **Tejveer Singh Anand**, IIT Delhi
P2-34	*Performance Enhancement of Parallel Flow Direct Contact Membrane Distillation using Localized Heating*, **Ravi Kumar Kandasamy**, IIT Delhi
P2-35	*Lightweight, Strong, Sustainable Graphene-Wood Composites as Aerospace Structural Materials*, **Afnan Elmubasher Malik**, Khalifa University
P2-36	*Optimization of Radiator Fin Geometry in Formula 1 Cars Using Machine Learning*, **Keshvi Singh**, IIT Delhi – Abu Dhabi
P2-37	*Molecular Modelling of the Gram-negative Bacterium Escherichia coli Cell Envelope*, **Jyoti Rai**, IIT Delhi – Abu Dhabi
P2-38	*Modulating Molecular Interaction in Deep Eutectic Solvent-Based Electrolytes Enables Enhanced Reactive CO_2 Capture*, **Mrityunjay Kumar Jha**, IIT Delhi – Abu Dhabi

TECHNICAL PROGRAM (Poster Sessions)

Wednesday, 17th December 2025	
Session	**Poster Session 3**
Room	Lobby, Fairmont Bab Al Bahr, Abu Dhabi
Poster No.	**Title**
P3-01	*Development of GIS-Based Maps and Change Detection for Groundwater Quality Assessment of Agra, Uttar Pradesh*, **Abhimanyu Verma**, IIT (BHU) Varanasi
P3-02	*Green Encapsulation of Metal Oxide and Noble Metal ZnO@Ag for Efficient Antibacterial and Catalytic Performance*, **Aisha Noor**, IIT Delhi
P3-03	*Investigating the Electrochemical Performance and Degradation Mechanism of $Na_3V_2(PO_4)_3$ for Sodium-Ion Batteries*, **Akshita Sharma**, IIT Delhi
P3-04	*Review: Bottlenecks of Indian Waste Management & AI Driven Solutions*, **Amna Rahman**, IIT Bombay
P3-05	*Unveiling Medium-Dependent Synergistic Role of Metals and Active sites in Prussian Blue Analogue-Derived FeCoTe for Hydrogen Evolution using Electroanalytical Techniques*, **Bhawna Rathor**, IIT Delhi
P3-06	*Biomass Briquettes as a Low-Carbon Alternative Fuel for Hard-to-Abate Industries*, **Bishakh Choudhury**, IIT Delhi
P3-07	*Design of Bend-Compensated Large Mode Area Fibers for Single-Mode High-Power Laser Systems*, **Soorej Thekkeyil**, IIT Delhi
P3-08	*Chew, Goldberger & Low equations: Eigensystem Analysis and Applications to One-Dimensional Test Problems*, **Chetan Singh**, IIT Delhi – Abu Dhabi
P3-09	*An Integrated Process-Structure-Property Model for Recycled Carbon Fibre Needlepunched Nonwovens: Towards Sustainable Structural Materials*, **Danvendra Singh**, IIT Delhi
P3-10	*Unveiling Chemical Evolution of Electrode-Electrolyte Interface in Sodium Ion Batteries from Machine Learning Potential-based Simulations*, **Dhananjay**, IIT Delhi
P3-11	*Impact of Geometry Structure on Hydrogen Desorption Behaviour in Metal Hydride Storage System*, **Gaurav Arora**, IIT Delhi
P3-12	*Assessment of Stability of Natural Colored Pigments in Indigenous Food Products*, **Gaurav Meena**, IIT Delhi
P3-13	*Hydrogen Storage Capacities in Nanoporous M2(m-dobdc) Metal-Organic Frameworks at Near Ambient Temperatures*, **Himani Joshi**, IIT Indore
P3-14	*Semi-Markov Modeling Based Reliability Analysis and Cost Optimization of Intelligent Transportation Systems Assisted with Cloud-Fog Server*, **Ishu Jain**, Netaji Subhas University of Technology Delhi
P3-15	*Integration of Solar Powered Distillation in Dairy Effluent Treatment*, **Ishwin Saini**, Heriot-Watt University
P3-16	*Resilient Pathways for Electricity and Emissions Futures in the United Arab Emirates: AI-Powered Predictive Modeling*, **Issa Zaiter**, Khalifa University
P3-17	*Multi-days Ahead Times Series Forecasting of Sea Surface Temperature using Transformer Models*, **Jayaram Valluru**, IIT Ropar
P3-18	*CO_2 Capture over Biomass Derived Porous Carbon Materials*, **Khushbu Bhavsar**, Sardar Vallabhbhai National Institute of Technology, Surat
P3-19	*Surface-Engineered Pd/g-C_3N_4 Catalysts for Light-Driven Formic Acid Dehydrogenation at Room Temperature*, **Mathivathani J R**, IIT Delhi

TECHNICAL PROGRAM (Poster Sessions)

Wednesday, 17th December 2025	
Session	**Poster Session 3**
Room	Lobby, Fairmont Bab Al Bahr, Abu Dhabi
Poster No.	**Title**
P3-20	*Process-level Evaluation of Adsorbents and Cycle Configurations for Post-Combustion CO_2 Capture*, **Mohammad Al Hamadi**, Khalifa University
P3-21	*Photonics to Physiology: BCN@CMC Nanocomposites for Optoelectronics and Biomedical Devices*, **Mohan Manjunathaswamy**, Khalifa University
P3-22	*From Bulk Solvents to Confined Spaces: Redefining Reaction Environments*, **Mohd Ussama**, IIT Delhi – Abu Dhabi
P3-23	*Eco-friendly Co-precipitation Processed $BaZn(VO_4)_2$ Nanoparticles as a Promising Anode Material for Li and Na-ion Batteries*, **Mohd Saqib**, IIT Delhi
P3-24	*AI-Augmented Socio-Technical Viability Framework for Multi-Criteria Evaluation of Energy Storage Technologies*, **Mohit Murarka**, IIT Delhi – Abu Dhabi
P3-25	*Efficient Simulation of Two-Dimensional Anisotropic Reaction–Diffusion Systems via Hybrid Cubic B-Spline Differential Quadrature: Applications to Tumor Growth Modeling*, **Nadeem Malik**, NSUT Delhi
P3-26	*AI-Driven Wind Resource Modeling for Efficient Wind-to-Hydrogen System Design at Jaisalmer*, **Nagasree Keerthi Pujari**, IIT Hyderabad
P3-27	*Performance Enhancement of Type IV Hydrogen Tanks Using Expanded Graphite*, **Omar El Khatib**, Khalifa University
P3-28	*Bridging Science and Policy: A Bibliometric Study of Nutritional Food Security in India*, **Pallavi Muwania**, Delhi Technological University
P3-29	*Exploring MOF – Hydrocarbon Integration for Sustainable Adsorption Cooling: An Accelerated Approach using Bayesian Optimization and Monte Carlo Simulations*, **S Muthukrishnan**, IIT Kanpur
P3-30	*Towards Generalizable ML-Based Molecular Dynamics: Challenges in Simulating Complex Minerals and Cementitious Materials*, **Sajid Mannan**, IIT Delhi
P3-31	*CO_2 Hydrogenation utilizing Pd/SBA-15 Catalyst: Identifying Scaling Behavior to Optimize Selectivity for CO and CH_4 Production*, **Sanket Bhumare**, National Chemical Laboratory Pune
P3-32	*Study of Drying Behavior of Multiple Sizes of Orthodox Tea Particle and CO_2 Reduction in Solar Drying for Small Tea Growers*, **Shantanu Kumar**, IIT Delhi
P3-33	*Synthesis of Butyl Butyrate as a Sustainable Aviation Fuel Using V_2O_5-Supported Silicomolybdic Acid Catalyst*, **Shariq Farhan Elahi**, Curtin University, Australia and IIT (ISM) Dhanbad, India
P3-34	*High-κ Interface Engineering for Energy-Efficient Spin–Orbit Torque Memories: A Materials Pathway Toward Digital Sustainability*, **Shubham Bhatt**, IIT Delhi
P3-35	*Concerted Photo and Chemical Ageing of Microplastics and its Transport Behaviour in Saturated Soil*, **Namita Das**, BITS Pilani Dubai
P3-36	Bridging Financial Inclusion and Climate Action: Sustainable Pathways for Mobile Financial Services, **Anuj Mohan Sherry**, Ericsson India Private Limited
P3-37	*Smart Thermal Management of Subsurface Pipelines for Hydrogen and District Energy Systems*, **Arjun Satheesh**, IIT Delhi – Abu Dhabi
P3-38	*Multiphysics Heat Transfer in Underground Energy Pipelines: Soil Conduction, Radiative Losses, and Materials-Led Efficiency Gains*, **Arjun Satheesh**, IIT Delhi – Abu Dhabi

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