



International Conference on
AI and Materials for Sustainability

15th-17th December, 2025

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	<p>Workshop 1</p> <p>Hands-on with Data-Driven Approaches to Accelerate Catalysis and Materials Research (Meta)</p> <p>Zachary W. Ullissi Meta Fundamental AI Research Rachit Khare Technical University of Munich</p>	<p>Workshop 2</p> <p>Why High-Quality Presentations and Posters Matter? (American Chemical Society)</p> <p>Ajay Jha Assistant Director, ACS Publications</p>
14:30 - 15:00	Coffee Break and Campus Tour	
15:00 – 17:00	<p>Workshop 3</p> <p>Innovation & Lab-to-Industry Pathways (American Chemical Society)</p> <p>Ajay Jha Assistant Director, ACS Publications</p>	<p>Workshop 4</p> <p>Research Data Management for Catalysis and Materials Research (NFDI4Cat and SPARC)</p> <p>Michael Libeau University of Leipzig Mohammad Khatamirad Technical University of Berlin Nikolaos G. Moustakas Leibniz Institute for Catalysis Rachit Khare Technical University of Munich</p>



International Conference on
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15th-17th December, 2025

Monday, 15th December 2025

Time	Venue: Fairmont Bab Al Bahr, Abu Dhabi				
07:30 - 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	<i>Powering the Change - Materials and Processes for Energy Transition</i> Johannes A. Lercher , Technical University of Munich				
10:00 – 10:30	<i>Multiscale Modeling for Accelerating Carbon Capture and Beyond</i> 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	<i>The Prospect of AI for Materials Discovery and Design of New Energy Materials</i> Jeffrey Snyder , Northwestern University				
11:30 – 12:00	<i>LIGHT, ELECTRONS and ACTION</i> Vivek Polshettiwar , Tata Institute of Fundamental Research				
12:00 – 12:30	<i>AI for Science and Sustainability: A Journey from Process Systems Engineering</i> 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	<i>TBD</i> Maryam Al Nahyan , New York University Abu Dhabi				
14:00 – 14:30	<i>Nature-Inspired Engineering of Functional Materials via a Systematic Design Methodology</i> Marc-Olivier Coppens , University College London				
14:30 – 15:00	<i>Discovering Reaction Networks and Life Cycle Pathways for a Sustainable Circular Economy of Chemicals</i> Bhavik Bakshi , Arizona State University				
15:00 – 15:30	<i>Hybrid Energy Systems: Innovative Research Pathways for Alleviating Global Energy Poverty</i> 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)				



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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	<i>Energy Security: Molecular Insight to Industrial Impact. Bringing Speed and Scale to Science for Sustainability</i> Ramakrishna R. Sonde , BITS Pilani, Goa Campus				
08:30 – 09:00	<i>ML Guided Catalyst Discovery for the Direct Hydrogenation of CO₂ to Jet Fuel</i> Jorge Gascon , King Abdullah University of Science and Technology				
09:00 – 09:30	<i>Designing Materials for Sustainability from First Principles</i> Shobhana Narasimhan , Jawaharlal Nehru Center for Advanced Scientific Research				
09:30 – 10:00	<i>2D Nanocomposite Membrane Engineering: A Journey from Research to Production</i> 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	<i>Machine Learning Models Across Chemistry and Materials</i> Zachary W. Ulissi , Meta Fundamental AI Research				
11:00 – 11:30	<i>Fathoming the Complexities of Reactions at Solid-Liquid Interfaces</i> David Flaherty , Georgia Institute of Technology				
11:30 – 12:00	<i>AI for Sustainability: Foundation Models for Closed-Loop, Knowledge-Driven Chemical Discovery and Process Optimization</i> Xiaonan Wang , Tsinghua University				
12:00 – 12:30	<i>Materials for Energy from Advanced Modeling</i> 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	<i>Protonic Ceramic Electrochemical Cells: Status and Outlook</i> Sossina M. Haile , Northwestern University				
14:00 – 14:30	<i>Scalable Production of Nanostructured Materials for Energy and Health Applications using Gas Phase Deposition</i> Ruud van Ommeren , Delft University of Technology				
14:30 – 15:00	<i>AI for Materials Driven Innovation for a Regenerative Economy</i> 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				



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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 <i>Sustainable Chemical Processes</i> Venue: Saqr Ballroom 1	Parallel Session 8 <i>AI for Sustainability II</i> Venue: Saqr Ballroom 2	Parallel Session 9 <i>Materials for Sustainability II</i> Venue: Saqr Ballroom 3	YRS Session 3 <i>Catalysis and Carbon Capture</i> Venue: Al Reem	YRS Session 4 <i>Water-Energy-Climate</i> 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	<i>Materials Science and Systems Innovation for the Just Energy Transition</i> Daniel M. Kammen , Johns Hopkins University				
11:00 – 11:30	<i>Decarbonising the Future: CCU and Hydrogen Landmark Redefining the Future of Energy</i> Kamal K. Pant , Indian Institute of Technology Roorkee				
11:30 – 12:00	<i>Decarbonising Heavy Industries: The Roles of Carbon Capture and Hydrate-Based Storage</i> Moses Tade , Curtin University				
12:00 – 12:30	<i>All Wastes are not Equal for Hydrogen Production via Gasification</i> 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	<i>Flame Aerosol Synthesis of High-Entropy Catalysts for Sustainability</i> Mark T. Swihart , University at Buffalo				
14:00 – 14:30	<i>Engineering Human+AI Collaboration for Process Safety and Sustainability Applications</i> Rajagopalan Srinivasan , Indian Institute of Technology Madras				
14:30 – 15:00	<i>Artificial Intelligence for Multiphase Reactors: Some Recent Advances</i> 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	<i>Computational Screening of Metallic and Mixed-metal Oxide Catalysts for Bio-oils Upgrading and H₂ Production</i> Lourdes Vega , Khalifa University				
16:00 – 16:30	<i>Outlook on Global Energy Transition: AI Catalysing Power Sector Transformation</i> Gauri Singh , International Renewable Energy Agency				
16:30 – 17:00	<i>Revisiting Energy Systems Modelling in the Context of AI</i> 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				



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TECHNICAL PROGRAM (Parallel Sessions 1 – 3)

Monday, 15 th December 2025			
Session	Parallel Session 1 <i>AI for Sustainable Chemical Processes</i>	Parallel Session 2 <i>Process Intensification for Sustainability</i>	Parallel Session 3 <i>Sustainable Materials for Energy Storage</i>
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 Sivaprasakash 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



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TECHNICAL PROGRAM (Parallel Sessions 4 – 6)

Tuesday, 16 th 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	<i>Computational Modeling and ML to Discover Materials and Reaction Pathways for Clean Energy Applications</i> Ananth Govind Rajan IISc Bangalore	<i>High-throughput Molecular and Process-level Screening of COFs for Carbon Capture via Pressure Swing Adsorption</i> Ashutosh Yadav IIT Jammu	<i>Engineering Polymer-surface Adhesion using Molecular Dynamics and Machine Learning</i> Divya Nayar IIT Delhi
15:50 – 16:10	<i>Zeolite-templated Carbon-based Air Electrodes for Lithium-Oxygen Battery</i> Maryam Khaleel Khalifa University	<i>Developing Nanostructured Catalysts for CO₂ Conversion using Density Functional Theory and Machine Learning</i> Sergey Kozlov NUS, Singapore	<i>Optimizing Renewable Energy and Thermal Storage with Advanced AI</i> Martin Takáč MBZUAI, Abu Dhabi
16:10 – 16:30	<i>Rational Design of Acidic Sites for Large Pore Zeolite for their Effective Utilization in Alkylation Reactions for Sustainable Aviation Fuel</i> Manjesh Kumar IIT Delhi	<i>Phonon Pathways to Green Energy: Thermoelectric Advances in 2D Chalcogenides</i> Nirpendra Singh Khalifa University	<i>Artificial Intelligence-Driven Optimization of Solid Oxide Electrolysis for Efficient Green Hydrogen Production</i> Munawar A. Shaikh UAE University
16:30 – 16:50	<i>Tunable Frameworks: Fit-to-Purpose Materials for Energy and Sustainability</i> Dinesh Shetty Khalifa University	<i>A Novel Carbon Capture and Utilization Technology to Recycle Heavy Metals from Industrial Waste</i> Vikram Singh IIT Delhi	<i>Development of Deep Learning based Bayesian Sensor Fusion Algorithms: Application to Hybrid Three Tank Experimental System</i> Jayaram Valluru IIT Ropar
16:50 – 17:10	<i>Bioplastics in Focus: Life Cycle Assessment and AI for a Greener Future</i> Suprakas Sinha Ray DSI - CSIR	<i>Computational-Guided Design of Functionalized Zeolite-Templated Carbons for Efficient CO₂ Capture</i> Daniel Bahamon Garcia Khalifa University	<i>Mapping the Elastic Properties of Sodium Silicate Glasses: A Simulation Pipeline Integrating SHIK and DeepMD with XGBoost for High-Fidelity Prediction</i> Hicham Jabraoui , TII
17:10 – 17:30	<i>Data-Driven Materials Designing for Optoelectronics</i> Dibyajyoti Ghosh IIT Delhi	<i>Climate Change, Sustainability and the Pathway Towards a Circular Economy: Global Perspectives and Challenges</i> Chithirai Pon Selvan Curtin University Dubai	<i>Machine Unlearning for Process Applications</i> Manoj Ramteke IIT Delhi



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TECHNICAL PROGRAM (Parallel Sessions 7 – 9)

Wednesday, 17th December 2025

Session	Parallel Session 7 <i>Sustainable Chemical Processes</i>	Parallel Session 8 <i>AI for Sustainability II</i>	Parallel Session 9 <i>Materials for Sustainability II</i>
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	<i>Direct Joule-Heated Membrane Reformer for On-Site Production of Ultra-pure Hydrogen</i> Rajesh Kumar Upadhyay IIT (BHU) Varanasi	<i>Artificial Intelligence – Driven Screening and Atomistic Simulation of Corrosion Inhibitors for Steel in Marine Environments</i> Shivraj Karewar Technology Innovation Institute	<i>Porous Organic and Coordination Polymer Materials for Energy and Environment Sustainability</i> Himanshu Aggarwal BITS Pilani, Hyderabad
08:20– 08:40	<i>Adsorption of Two Anionic Mordant Red Dyes by Differently Activated Plant Derived Biochar</i> Umesh Mishra NIT Agartala	<i>Prediction of Descriptor (CO and OH) Binding Energy on Cu-based Bimetallic Alloys using ML Approach</i> Shelaka Gupta IIT Hyderabad	<i>Microwave-Synthesized Graphene Quantum Dots as Hydrophilic Modifiers for High-Performance Polysulfone Ultrafiltration Membrane</i> Jagdeeshbabu P Ettiappan NITK Surathkal
08:40– 09:00	<i>Magnesium-CaNi Composite Systems for Hydrogen Storage Applications</i> Nitesh Kumar IIT Jammu	<i>Graph Neural Network Assisted Sensor Placement Design using Reliability Criteria</i> Om Prakash IIT Delhi	<i>Microarchitected Hierarchically Porous PLA/S/CNT Nano-composite Electrodes Enabled via 3D Printing with Remarkable Performance in Li-ion Batteries</i> Vinay Gupta Khalifa University
09:00– 09:20	<i>Deciphering the Role of Metals and Promoter Loading on CO_x Free Turquoise H₂ Production for Carbon Neutral Coal Mining</i> Ejaz Ahmad IIT (ISM) Dhanbad	<i>Deconstruction of Biomass for Bioenergy: Molecular Insights into Xylan-Cellulose Adhesion</i> Madhulika Gupta IIT (ISM) Dhanbad	<i>Core-shell Nanotechnology Assisted Nano-Composite Anode (Gr/Si@TiO₂) for Li-ion Battery</i> Deepak Kumar IIT Delhi
09:20– 09:40	<i>Radiation-based Techniques for Detailed Investigation of Cohesive Particle Flows to Make Advanced Materials</i> Ruud van Ommeren Delft University of Technology	<i>Tuning the Selectivity of Hydrogenation and C-C Coupling Pathways during Biomass Conversion</i> Rachit Khare Technical University of Munich	<i>Graphene Anti-Corrosion Coatings for Sustainable Infrastructure and Industrial Efficiency</i> Husain Kanchwala IIT Delhi



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TECHNICAL PROGRAM
(Young Researchers and Scientists Sessions)

Monday, 15th December 2025

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



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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	<i>Microwave-Assisted Synthesis of ZnFe₂O₄ Nanomaterials for High-Performance Supercapacitor Application</i> , Pavan Dhurandhar , University of Mumbai
15:40 – 15:50	<i>Engineering Sustainable Materials and Methods for Lightweight Lattice Structures</i> , Asha Viswanath , Khalifa University
15:50 – 16:00	<i>Export Competitiveness of Controlled Environment Saffron Production: Entrepreneurial Evidence from Indian Emerging States</i> , Sahiba Sharma , Manav Rachna University, Faridabad
16:00 – 16:10	<i>Morphological Engineering of CoFe₂O₄ Nanostructures for High-Performance and Durable Supercapacitor Electrodes</i> , Rukayat Zakari , Khalifa University
16:10 – 16:20	<i>From Nature to Power: Eco-Friendly Energy Scavenging and Self-powered Smart Sensing</i> , Bushara Fatma , Khalifa University
16:20 – 16:30	<i>Advanced Inorganic Materials for Energy Storage Devices</i> , Rohan Narkar , University Of Mumbai
16:30 – 16:40	<i>Electromagnetic Shielding Performance of Large Lateral-Sized Graphene Sheets</i> Shanavas Shajahan , Khalifa University



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TECHNICAL PROGRAM
(Young Researchers and Scientists Sessions)

Wednesday, 17th December 2025

Session	YRS Session 3 Catalysis and Carbon Capture
Room	AI Reem, Fairmont Bab Al Bahr, Abu Dhabi
Chairs	Ananth Govind Rajan, Manjesh Kumar
08:00 – 08:10	<i>Selective Formation of Formic Acid via Low-Temperature Methane Oxidation on Au-Fe/Na-ZSM-5: Experimental and DFT Insights</i> , Iqra Ahangar , Higher Colleges of Technology, Abu Dhabi
08:10 – 08:20	<i>Ni-Ru Catalysts for Biogas Reforming: Mitigating Carbon and Sulfur Induced Deactivation via MoO₃ Promotion</i> , Satyajit Panda , Council of Scientific & Industrial Research, Dehradun
08:20 – 08:30	<i>Facile Hydrothermal Synthesis of MoS₂/MXene Composite for Efficient Rhodamine B Dye Adsorption from Aqueous Solutions</i> , Riddhi Patel , Pandit Deendayal Energy University, Gandhinagar
08:30 – 08:40	<i>Synthesis-dependent function of Pd/CHA Zeolites under Cold-start conditions: An Operando FT-IR Spectroscopy and Microreactor Study</i> , Yusra Hamid , University of Lisbon
08:40 – 08:50	<i>Nonpolynomial Spline Approach for CO₂ Adsorption–Diffusion Modelling</i> , Kirandeep Kaur , Netaji Subhash University of Technology Delhi
08:50 – 09:00	<i>Integrated Experimental, Simulation, and Process-level Evaluation of Advanced Adsorbents for PSA-based CO₂ Capture in Cement Plants</i> , Khushboo Yadava , Grihitum, IIT Mandi Catalyst
09:00 – 09:10	<i>Photocatalytic Degradation of Sulfamethoxazole with TiO₂-Fe₂O₃ Photocatalyst under Solar Light Irradiation</i> , Jitendra Pal Salavadhi , NITK, Surathkal
09:10 – 09:20	<i>Conformational Dynamics of O-2 Acetylated Xylan on Cellulose Surfaces: Implications for Sustainable Biofuel Production</i> , Tripti Kundu , IIT (ISM) Dhanbad
09:20 – 09:30	<i>Barriers for Integrating Carbon Capture and Storage into Net-Zero Pathways: A Comprehensive Literature Review</i> , Priji Biju , The British University in Dubai



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



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



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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	<i>Hydrogen Storage Capacities in Nanoporous M2(m-dobdc) Metal-Organic Frameworks at Near Ambient Temperatures, Himani Joshi, IIT Indore</i>
15:35	<i>From Bulk Solvents to Confined Spaces: Redefining Reaction Environments, Mohd Ussama, IIT Delhi – Abu Dhabi</i>
15:40	<i>Photonics to Physiology: BCN@CMC Nanocomposites for Optoelectronics and Biomedical Devices, Mohan Manjunathaswamy, Khalifa University</i>
15:45	<i>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</i>
15:50	<i>Novel Tri-Amine Blend for Efficient Post-Combustion CO₂ Capture: Experimental Absorption-Desorption Studies, Kinetic Analysis, Modeling, and Spectroscopic Investigations, Akhil Kumar Gupta, IIT (BHU) Varanasi</i>
15:55	<i>Investigating the Electrochemical Performance and Degradation Mechanism of Na₃V₂(PO₄)₃ for Sodium-Ion Batteries, Akshita Sharma, IIT Delhi</i>
16:00	<i>An Integrated Process-Structure-Property Model for Recycled Carbon Fibre Needle Punched Nonwovens: Towards Sustainable Structural Materials, Danvendra Singh, IIT Delhi</i>
16:05	<i>Surface-Engineered Pd/g-C₃N₄ Catalysts for Light-Driven Formic Acid Dehydrogenation at Room Temperature, Mathivathani J R, IIT Delhi</i>
16:10	<i>Eco-friendly Co-precipitation Processed BaZn(VO₄)₂ Nanoparticles as a Promising Anode Material for Li and Na-ion Batteries, Mohd Saqib, IIT Delhi</i>
16:15	<i>Green Encapsulation of Metal Oxide and Noble Metal ZnO@Ag for Efficient Antibacterial and Catalytic Performance, Aisha Noor, IIT Delhi</i>
16:20	<i>Synthesis of Butyl Butyrate as a Sustainable Aviation Fuel Using V₂O₅-Supported Silicomolybdic Acid Catalyst, Shariq Farhan Elahi, Curtin University, Australia and IIT (ISM) Dhanbad, India</i>
16:25	<i>Interfacial Charge Transfer Dynamics in Electrochemical CO₂ Reduction on Gold Electrodes: Influence of Ionic Strength and Cation Identity in Na₂CO₃-Based Electrolytes, Jagriti Malik, IIT Delhi</i>
16:30	<i>Biomass Briquettes as a Low-Carbon Alternative Fuel for Hard-to-Abate Industries, Bishakh Choudhury, IIT Delhi</i>
16:35	<i>Exploring MOF – Hydrocarbon Integration for Sustainable Adsorption Cooling: An Accelerated Approach using Bayesian Optimization and Monte Carlo Simulations, S Muthukrishnan, IIT Kanpur</i>
16:40	<i>High-κ Interface Engineering for Energy-Efficient Spin-Orbit Torque Memories: A Materials Pathway Toward Digital Sustainability, Shubham Bhatt, IIT Delhi</i>
16:45	<i>Unexpected Lowering of Charge-Transfer Resistance in Ultra-Long Cycled (>30,000 Cycles) Solution-Processed Laminar-Crystalline Li₃VO₄ Anodes and its Li₃VO₄ LFP Full Cells Performance in 18650 form factor, Tejveer Singh Anand, IIT Delhi</i>
16:50	<i>Techno-Economic Analysis of Green Hydrogen Project in Abu Dhabi, Adnan Nagah, Abu Dhabi National Oil Company (ADNOC) and IIT Delhi – Abu Dhabi</i>