

SCIENTIFIC PROGRAMME

2nd DAE Symposium on Advances in Atomistic and Continuum Modeling (DAE-SAACM 2026)

Venue: Multipurpose Hall (MPH), Anushaktinagar, Mumbai | 19 – 21 November 2026

PRE-REGISTRATION · Wednesday, 18 November 2026

16:30 – 18:30	**Pre-registration**

DAY 1 · Thursday, 19 November 2026

08:00 – 10:00	**Registration**
09:00 – 09:45	**Inauguration**
09:45 – 10:00	**HIGH TEA**

SESSION I | Chair: **Prof. Swapan K Ghosh**

10:00 – 10:30	**Prof. Swapan Pati** | JNCASR, Bangalore *Computational Modeling of Materials for Applications in Energy Conversion and Storage*	PL1 · N
10:30 – 10:50	**Prof. Manoj K Warrier** | BARC, Mumbai *Multi-scale Investigation of Helium Transport and Clustering in Tungsten*	IL1 · I
10:50 – 11:10	**Prof. Rajaraman Ganesh** | IPR, Gandhinagar *Multiscale challenges in thermonuclear plasmas confined in Tokamaks*	IL2 · N
11:10 – 11:20	**MINI TEA**	

SESSION II | Chair: **Prof. P. Modak, Prof. A. K. Arya**

11:20 – 11:40	**Prof. S. Karmakar** | TIFR, Hyderabad *Tunable Yielding and Emergent Rheology in Amorphous Solids with Active Particle Doping*	IL3 · E
11:40 – 12:00	**Dr. Tarak Patra** | IIT, Chennai *From Bond-Exchange Kinetics to Polymer Miscibility: A Multiscale Modeling Framework*	IL4 · E
12:00 – 12:20	**Prof. Abhijit Chatterjee** | IITB, Mumbai *Solid-state hydrogen storage and purification: Multiscale insights into coupled size-chemo-thermo-mechanical effect in hydride phase diagram to growth rate*	IL5 · D
12:20 – 12:40	**Dr. Indrajit Tah** | CGCRI, Kolkata *Physics-Informed Graph Neural Networks for Predicting Mechanical Failure in Disordered Materials*	IL6 · H

12:40 – 13:00	**Prof. Amrita Bhattacharya** | IITB, Mumbai *Double-Exchange Ferromagnetism and A-Site-Disorder-Driven Inhomogeneity in Monovalent K-Doped LaMnO3*	IL7 · N
13:00 – 14:00	**LUNCH**	
SESSION III | Chair: **Prof. A.K. Dureja, Prof. K.K. Singh**		
14:00 – 14:30	**Prof. A.W. Patwardhan** | ICT, Mumbai *Design of Gas Inducing Impellers*	PL2 · K
14:30 – 14:50	**Dr. Sanjeev Kumar Sharma** | NPCIL, Mumbai *Containment Spray System Modelling, validation and analysis for 700 MWe Indian PHWR Containment*	IL8 · M
14:50 – 15:10	**Dr. Priyanshu Goyal** | BARC, Mumbai *CFD in Nuclear Safety*	IL10 · K
15:10 – 15:30	**Dr. Saurav Sarkar** | BARC, Mumbai *A Multi-Stage Simulation Framework for Drop at Interface Coalescence*	IL11 · J
15:30 – 15:42	**Mr. Sukhdeep Singh** | BARC, Mumbai *Prediction of mixing time in external loop airlift reactors using Extreme Gradient Boosting*	CL1 · H
16:00 – 16:15	**TEA**	
SESSION IV | Chair: **Prof. Jayant Singh**		
16:15 – 16:35	**Dr. R. Venkat Ramani** | TIFR, Mumbai *Simulations and Spectral Deconvolution of Protein Charge Transfer Spectra*	IL12 · G
16:35 – 16:55	**Prof. Jagannath Mondal** | TIFR, Hyderabad *Integrating artificial intelligence with computer simulation & Experiment*	IL13 · H
16:55 – 17:15	**Prof. Sudip Das** | SINP, Kolkata *Physics-Informed Machine Learning for Enzyme Catalysis*	IL14 · H
17:15 – 17:27	**Dr. Debashree Chakraborty** | NIT, Karnataka *Free energy calculations for the permeation process of Cell Penetrating Peptides*	CL2 · G
SESSION V		
17:30 – 18:30	**Poster Presentation (P1 – P32)**	
18:30 – 19:00	**SACM Annual General Body Meeting**	
20:00 – 22:00	**BANQUET DINNER**	

DAY 2 · Friday, 20 November 2026

SESSION VI | Chair: **Prof. N. Choudhury**

09:15 – 09:45	**Prof. J.K. Singh** | IIT, Kanpur *AI-Driven Materials Discovery for Sustainable Technologies*	PL3 · H
09:45 – 10:15	**Prof. Jhumpa Adhikari** | IITB, Mumbai *Molecular insights into the influence of additives on gas hydrate dissociation*	PL4 · N
10:15 – 10:35	**Prof. Snehashis Daschakraborty** | IIT, Patna *CO2 Adsorption in Humid COFs: A Transition Matrix Monte Carlo Study*	IL15 · G
10:35 – 10:55	**Prof. Santosh Mogurampelly** | IIT, Jodhpur *Beyond Stokes-Einstein: Power Laws, Ion-Pair Relaxation, and Ion Transport in Biopolymer Electrolytes*	IL16 · G

11:00 – 11:15 TEA

SESSION VII | Chair: **Prof. D.V. Udupa**

11:15 – 11:35	**Dr. Supratim Majumdar** | BARC, Mumbai *Engineering the Quantum State: Hardware and Control for Superconducting Qubits*	IL17 · H
11:35 – 11:55	**Dr. Rahul Maitra** | IIT, Mumbai *Quantum-Centric Supercomputing via Physics-Informed Generative Wavefunction Reconstruction and Adaptation to Distributed Architecture*	IL18 · H
11:55 – 12:15	**Dr. Yamijala SRK Chaitanya** | IIT, Chennai *Simulating Chemical Reaction Dynamics Using Sample-Based Quantum Diagonalization: A Quantum-Centric Supercomputing Approach*	IL19 · H
12:15 – 12:35	**Dr. Sandip Joshi** | BARC, Mumbai *Quantum Simulation with Superconducting Qubits*	IL20 · H
12:35 – 12:55	**Dr. Urvashi G.K.** | BARC, Mumbai *Transforming Computational Modelling through Artificial Intelligence and Machine Learning*	IL21 · H

13:00 – 14:00 LUNCH

PARALLEL SESSIONS · 14:00 – 16:00

SESSION VIII-A | Chair: **Prof. D.K. Maity, Prof. Madhumita Goswami** | Venue: **MPH**

14:00 – 14:12	**Mr. Vashishtha Patel** | IIT, Mumbai *Machine Learning Accelerated Density Functional Theory Approach for Predicting Activation Barriers and Reaction Pathways in Methane-to-C2 Conversion*	CL3 · H
14:12 – 14:24	**Ms. Janvi Semwal** | THDC Institute, Tehri *Kaṇēyana: Generative Phase-Space Propagation to Accelerate MD of Defect Transport and Interactions*	CL4 · H
14:24 – 14:36	**Prof. Srikanth Divi** | MIT, Mahe *Multiscale Computational Investigation of Functionalized Boron Nitride Nanotubes for Enhanced Hydrogen Storage*	CL5 · D

14:36 – 14:48	**Ms. Mahima Patel** | Institute of Science, Mumbai *Density Functional Theory and Machine Learning-assisted Screening of Li-decorated C20 and its B- and N-substituted derivatives for gas sensing*	CL6 · H
14:48 – 15:00	**Mr. Subhom Ghosh** | JNCASR, Bengaluru *MACE-GEN: A Generalized Score-Based Diffusion Framework for Amorphous Materials*	CL7 · H
15:00 – 15:12	**Mrs. Anindita Sarkar** | BARC, Mumbai *Studying the change in structural, mechanical and electronic properties of Pmmn-phase of U2Mo alloy through Nb and Zr doping: Insights from Density Functional Theory*	CL8 · B
15:12 – 15:24	**Dr. Vijay Lamba** | Gurugram University *Modelling of Charge Transport in Thiophene Nanowires: Length Dependent Transition from Coherent Tunnelling to Thermally Activated Hopping*	CL9 · G
15:24 – 15:36	**Mr. Debendra Meher** | JNCASR, Bengaluru *Insights into Zinc-Doped Sodium Borosilicate Glass Modelled Using Machine Learned Potentials*	CL10 · E
15:36 – 15:48	**Dr. Sachin Kumar** | BARC, Mumbai *Fractional Magnetization Plateaus and Quantum Phase Transitions in Spin-1/2 Heisenberg Spin Chain*	CL11 · N
15:48 – 16:00	**Ms. Km Chanchal** | BARC, Mumbai *Lattice dynamics as a descriptor of superionic diffusion in solid electrolytes*	CL12 · H

SESSION VIII-B | Chair: **Prof. T. K. Ghanty, Prof. K.R.S. Chandrakumar** | Venue: **Conference Room, TSH**

14:00 – 14:12	**Mr. Aaditya Majalee** | BARC, Vizag *Molecular Dynamics Simulations of collision cascades in Zirconium using ADP and EAM potentials*	CL13 · F
14:12 – 14:24	**Mr. Akash Meel** | IIT, Jodhpur *Revisiting the Stokes-Einstein relation in biopolymer electrolytes*	CL14 · E
14:24 – 14:36	**Dr. Srinivasagopalan Madhavan** | BARC, Vizag *Coupled MD-HD Multiscale Framework for Shock-Induced Spall Fracture in FCC Polycrystals*	CL15 · N
14:36 – 14:48	**Dr. Ravi Chandra Dutta** | IIT, Dharwad *Molecular-Level Understanding of Gas Transport in COF-Based Mixed Matrix Membranes: The Role of the Polymer-Filler Interface*	CL16 · C
14:48 – 15:00	**Dr. Sachin MB Gautham** | IISc, Bengaluru *Copolymer Sequence and Filler Chemistry Control the Interfacial Glass Transition in Acrylic–Polystyrene Paint Nanocomposites*	CL17 · E
15:00 – 15:12	**Mr. Sumanth Madivada** | HBNI, Mumbai *CFD modelling of pulsatile flow in a cylindrical vessel with a central pulse leg*	CL18 · G
15:12 – 15:24	**Dr. Shivanand Kumar Veesam** | NIT, Calicut *Structural and Thermodynamic Screening of MOFs for Competitive I2 and CH3I Capture across Variable Nuclear-Reprocessing Off-Gas Conditions*	CL19 · C
15:24 – 15:36	**Dr. Anjana Tripathi** | IITB, Mumbai *Coverage-Driven Machine Learning Framework for the Rational Design of High-Entropy Alloy Electrocatalysts*	CL20 · H
15:36 – 15:48	**Mr. Adwait Karkare** | ICT, Mumbai *Numerical Assessment of Sub-Cooled Flow Boiling in a Helical Coil using OpenFOAM*	CL21 · K

15:48 – 16:00	**Mr. Kshitij Acharya** | HBNI, Mumbai *A Modernized CPL Library for concurrent Molecular Dynamics-Continuum Coupling: Verification and Extension to Reactor Thermal Hydraulics*	CL22 · I

16:00 – 16:15 TEA

SESSION IX | Chair: **Prof. Jhumpa Adhikari**

16:15 – 16:35	**Prof. Ateeque Malani** | IIT Bombay *Molecular Understanding of Radionuclide Adsorption and Immobilization in Clay Minerals: Surface and Nanopore Interactions*	IL22 · A
16:35 – 16:55	**Prof. Achintya Datta** | IITB, Mumbai *Including Relativistic Effects in Quantum Chemistry Calculations*	IL23 · B
16:55 – 17:15	**Dr. Debashish Kundu** | ICT, Jalna *Systematic Exploration of COSMO-SAC-PDH Model for Rare Earth Element Leaching in Deep Eutectic Solvents*	IL24 · A
17:15 – 17:35	**Dr. A. Das** | BARC, Mumbai *Reverse Migration of Competing Metal Ions from Organic Phase to Aqueous Phase Using Molecular Dynamics Simulations*	IL25 · C

SESSION X

17:35 – 18:35 Poster Presentation by Participants (P33 – P65)

SESSION XI · INDUSTRY PRESENTATIONS | Chair: **Kumar Vaibhav**

18:35 – 18:45	**Micro Point Computers Pvt. Ltd**	IP1
18:45 – 18:55	**Materials Design**	IP2
18:55 – 19:05	**CADFEM India Pvt. Ltd**	IP3
19:05 – 19:15	**DHIO Research and Engineering Pvt. Ltd**	IP4

20:00 – 22:00 BANQUET DINNER

DAY 3 · Saturday, 21 November 2026

SESSION XII | Chair: **Prof. Swapan Pati**

09:15 – 09:35	**Prof. G.P. Das** | TCG Crest *The DFT-ML Alliance for Next-Generation Battery Materials*	IL26 · H
09:35 – 09:55	**Dr. Sharat Chandra** | IGCAR, Kalpakkam *Development of suitable machine learned interatomic potentials for studying diffusion in FeCr-H and IPG systems*	IL27 · H
09:55 – 10:15	**Dr. Debjani Karmakar** | BARC, Mumbai *Exotic quantum phases: impact of dynamical correlation and magnetism*	IL28 · H
10:15 – 10:35	**Dr. Naiwrit Karmodak** | SNU, Delhi *Design principles of Single-Atom Catalysts for electrocatalytic applications*	IL29 · D
10:35 – 10:55	**Dr. Arjun Pradeep** | IGCAR, Kalpakkam *From Multiphase Modelling to Experimental Investigation of Fission-Product Transport in Sodium-Cooled Fast Reactors*	IL30 · N

11:00 – 11:15 TEA

SESSION XIII | Chair: **Prof. Manoj Warrier**

11:15 – 11:35	**Prof. Utpal Sarkar** | Assam University *Machine learning approach to screen potential material: Insights from chemical reactivity*	IL31 · H
11:35 – 11:55	**Dr. Pooja Sahu** | BARC, Mumbai *A Multiscale DFT, AIMD, MD and Bayesian Optimization Framework for Accurate Prediction of Uranyl Extraction in Aqueous-Organic Biphasic Systems*	IL32 · C
11:55 – 12:15	**Dr. Mayank Gupta** | BARC, Mumbai *Machine-Learned Molecular Dynamics for Understanding Ion and Thermal Transport in Energy Materials*	IL33 · G
12:15 – 12:35	**Dr. Sudarshan Vijay** | IIT, Mumbai *Fewer calculations, same answers: universal machine learning potentials as a guide for density functional theory*	IL34 · H
12:35 – 12:55	**Dr. Gopakumar** | IGCAR *Computational Chemistry for f-Element Separation*	IL35 · B

13:00 – 14:00 LUNCH

SESSION XIV | Chair: **Prof. Ranjan Mittal**

14:00 – 14:20	**Dr. B Chakraborty** | BARC, Mumbai *Defect, Doping & Strain: Tools to design materials for Energy Storage, Spintronic & Electrocatalytic Applications*	IL36 · D
14:20 – 14:40	**Utkarsh Bharadwaj** | BARC, Vizag *Towards Predictive Atomistic Modelling of Radiation Damage: Advances in Potentials, Defect Analysis and Dynamics*	IL37 · H

14:40 – 14:55	**Dr. Anil Boda** | BARC, Mumbai *Electronic Structure, Phonon Dynamics, and Thermal Transport Properties of Metallic Uranium Isotopes: Density Functional Theory and Boltzmann Transport Equation based Explorations*	ISL1 · A
15:00 – 15:15	**TEA**	

SESSION XV | Chair: **Prof. C. Majumder**

15:15 – 15:35	**Prof. Susmita Roy** | IISER, Kolkata *STEM: A Structural-Topology-based Electrostatic Model of RNA*	IL38 · N
15:35 – 15:55	**Dr. Arup Pathak** | BARC, Mumbai *Structure and Dynamics of Heavy Metal Binding to Serum Protein*	IL39 · N
15:55 – 16:10	**Dr. D. Bandyopadhyay** | BARC, Mumbai *DFT-Based QSAR Modelling for Toxicity Prediction of Nuclear Solvent Extractants: Towards Safer Solvent Systems*	ISL2 · A
16:10 – 16:25	**Dr. Yogendra Kumar** | IISc, Bengaluru *Engineering Nanostructured Materials for Uranyl Ion Extraction: From Selective COF Membranes to PAMAM-Based Adsorbents*	ISL3 · A
16:25 – 16:40	**Dr. Srinivasu K** | BARC, Mumbai *Exploring 2D Conjugated MOF based Single-Atom Catalysts for Energy Related Applications*	ISL4 · D

SESSION XVI | Chair: **Shri Kalyan Bhanja, Shri K.T. Shenoy, Prof. Sk. Musharaf Ali**

16:45 – 17:30	**Panel Discussions, Award Distribution, Feedback and Concluding Session**
	Vote of Thanks

LECTURE TYPES & THEMES

Code	Lecture type	Number	Duration
PL	Plenary Lecture	4	30 min
IL	Invited Lecture	38	20 min
ISL	Invited Short Lecture	4	15 min
CL	Contributed Lecture	22	12 min
IP	Industry Presentation	4	10 min

Theme	Theme title
A	Computational Thermodynamics of Nuclear Materials
B	Density Functional Theory Based Modeling of Lanthanides-Actinides
C	Molecular Modeling of Chemical Separation Processes
D	Atomistic Modeling of Catalyst and Design of Hydrogen Storage Materials
E	Atomistic Modeling of Multi-Component Glass and Rechargeable Battery
G	Theory and Computation on Molecular Transport Phenomena and Spectroscopy
H	ML-AI and Quantum Computing Accelerated Computational Modeling
I	Multiscale Modeling of Reactor Materials
J	CFD and Mathematical Modeling for Applications in Nuclear Fuel Cycle
K	Applications of CFD and Mathematical Modeling in Thermal Hydraulics
M	Continuum Modeling in Nuclear Reactor Technology
N	Modeling Driven Experiments or Experiments Driven Modeling