

Program Schedule of DAE-SAACM-2024

DAE Convention Centre, Anushaktinagar

Day 0 (22 October, Tuesday, 2024)					
Pre-registration (17:00-19:00hrs)					
Day 1 (23 October, Wednesday, 2024)					
Registration (08:00-09:45hrs)					
Inauguration (09:00-09:50hrs)					
Welcome Address	:	Dr. Sulekha Mukhopadhyay, Head, ChED	:	09:00-09:05hrs	
Introductory Remarks	:	Dr. R. Tewari, Director, MG	:	09:05-09:10hrs	
Address 1	:	Shri K. T. Shenoy, Director, ChEG & Chairman, OC	:	09:10-09:20hrs	
Chief Guest Address	:	Prof. R. B. Grover, Member, Atomic Energy Commission & Founding Director, HBNI	:	09:20-09:35hrs	
Guest of Honor	:	Prof. E. D. Jemmis, IISc, Bangalore	:	09:35-09:45hrs	
Vote of Thanks	:	Dr. Sk. Musharaf Ali, Convener, OC	:	09:45-09:50hrs	
National Anthem					
Group Photo					
High Tea: 09:55 - 10:25hrs					
Session-I (main) (10:30-11:55hrs)					
(Chair: Prof. Swapan K. Ghosh, Dean, CEBS & Prof. D. K. Maity, Associate Dean, HBNI)					
PL-1		Prof. E. D. Jemmis, IISc, Bangalore (<i>Borophenes, Borophites and An Extended Rudolph Diagram</i>)	:	10:30-11:00hrs	
PL-2		Prof. P. K. Maiti, IISc, Bangalore (<i>Charge transport in the D2 branch of Photosystem II and Electrical conductance of DNA and RNA</i>)	:	11:00-11:30hrs	
EIL		Dr. Pooja Sahu, BARC, Mumbai (<i>Atomistic to continuum Hybrid Simulation Models</i>)	:	11:30-11:55hrs	
Session-II (main) (12:00-12:50hrs)					
(Chair: Prof. Satrajit Adhikari, IACS, Kolkata)					
IL-1		Prof. Pranab Sarkar, Visva Bharati, Shantiniketan (<i>Designing Functional Materials for Sustainable Energy</i>)	:	12:00-12:25hrs	
IL-2		Dr. A. Banerjee, RRCAT, Indore (<i>Development of Neural Network-based Pauli potential for the Advancement of Orbital-Free Density Functional Theory</i>)	:	12:25-12:50hrs	
Lunch break: 12:55-13:55hrs					
Session-III (14:00-16:00hrs)					
Parallel-A (main) (Chair: Dr. Rajesh, K., Head, CD)			Parallel-B (mini) (Chair: Dr. R. N. Singh, Head, MMG)		
IL-3	Dr. Manoj Warrior, BARC, Vizag (<i>Connecting displacements per atom to the morphology of defects in radiation damage</i>)	14:00-14:25 hrs	IL-5	Dr. Amrit Prakash, BARC, Mumbai (<i>Fabrication of Fast Reactor Fuels and their Characterisation</i>)	14:00-14:25 hrs

IL-4	K. Vaibhav, BARC, Mumbai (Anupam Supercomputers: Evolving to adopt changing computational requirements and paradigms)	14:25-14:50 hrs	IL-6	Dr. Abhijit Ghosh, BARC, Mumbai (Effect of green density and composition of preform on final density of reaction bonded silicon carbide)	14:25-14:50 hrs
ISL-1	Vibhuti Duggal, BARC, Mumbai (Brain Segmentation using Deep Learning)	14:50-15:10 hrs	IL-7	Dr. Madhumita Goswami, BARC, Mumbai (Glass/Glass-ceramics: An Inevitable Material for Emerging Technology)	14:50-15:15 hrs
ISL-2	Dr. A. Boda, BARC, Mumbai (Machine Learning based design of solvent-liagnd system)	15:10-15:30 hrs	ISL-4	Dr. Malay K. Rana, IISER, Berhampur (Rapid Discovery of Advanced Porous Materials for CO ₂ capture and Hydrocarbon Storage/Separation)	15:15-15:35 hrs
ISL-3	Dr. Anirban Mondal, IIT, Gandhinagar (Active Learning-Driven Force Field Parameterization for Electrolyte Systems in Battery Applications)	15:30-15:50 hrs	ISL-5	Dr. A. K. Singha Deb, BARC, Mumbai (Computational Chemistry Aided Experimental Strategies for Isotope Separation of Zinc)	15:35-15:55 hrs
Tea Break: 16:00-16:25hrs					
Session-IV (16:30-18:20hrs)					
Parallel-A (main) (Chair: Dr. Soumya Adhikari, Director, KMG)			Parallel-B (mini) (Chair: Dr. Aditi Ray, Head, ThPS)		
IL-8	Dr. Achintya Kumar Dutta, IIT, Bombay, Mumbai (Secondary Electron Attachment Induced Radiation Damage to Genetic Materials)	16:30-16:55 hrs	IL-9	Dr. Amrita Bhattacharya, IITB, Mumbai (In search of spin orbit driven ferroelectric Rashba switches in Perovskite oxides)	16:30-16:55 hrs
ISL-6	Dr. Sangita Sen, IISER, Kolkata (Theoretical modelling of strongly correlated excited states of INVEST OLED molecules)	16:55-17:15 hrs	IL-10	Dr. Debjani Karmakar, BARC, Mumbai (Kagome Superconducting Series AV ₃ Sb ₅ (A = Cs, Rb, K): interplay of magnetism, superconductivity and charge-order)	16:55-17:20 hrs
ISL-7	Dr. A. Das, BARC, Mumbai (Understanding of Interfacial Properties in Presence of Polar and Nonpolar Solvents - Insight from Molecular Dynamics Simulations)	17:15-17:35 hrs	ISL-10	Dr. Santosh Mogurampelly, IIT, Jodhpur (Ionic Conductivity Mechanisms in Liquid Electrolytes)	17:20-17:40 hrs

ISL-8	Dr. D. Bandyopadhyay, BARC, Mumbai (Investigation of water-alcohol/aldehyde interface to explore the structure, dynamics and accumulation of self-ions at the interface by using Molecular Dynamics Simulation)	15:35-17:55 hrs	ISL-11	Dr. B. Chakraborty, BARC, Mumbai (Exciting Properties of 2D Nanomaterials & Their Applications for Energy Storage & Sensing Applications: Perspectives From quantum Simulations)	17:40-18:00 hrs
ISL-9	Dr. Arunasis Bhattacharya, BARC, Mumbai (Computational Chemistry to unfold the Complexation/Extraction behaviour of the 'f' block elements)	17:55-18:15 hrs	ISL-12	Dr. Naiwrit Karmadok, SNIE, Delhi NCR (Multiscale Modelling of the Stability and Catalytic Activity of Materials for sustainable energy resources)	18:00-18:20 hrs
Banquet Dinner (20:00-22:00hrs) at Oasis, Deonar					
Felicitation to Prof. D. K. Maity and Dr. A. K. Arya					
Day 2 (24 October, Thursday, 2024)					
Session-V (main) (09:30-10:50hrs) (Chair: Dr. Niharendu Choudhury, Head, ChD)					
PL-3	Prof. Swapan Pati, JNCASR, Bangalore (<i>Computational Modelling of a few Homogeneous and Heterogeneous Catalytic Reactions</i>)	:			09:30-10:00hrs
IL-11	Prof. Ajay Chaudhari, Institute of Science, Mumbai (<i>Metal decorated materials for hydrogen storage : A Density Functional Theory approach</i>)	:			10:00-10:25hrs
IL-12	Dr. Sk. Musharaf Ali, BARC, Mumbai (Atomistic Modeling Strategy for Evaluation of Properties of Molecular System in Atomic Energy Applications)	:			10:25-10:50hrs
Tea break (10:55-11:25hrs)					
Session-VI (main) (11:25-13:05hrs) (Chair: Dr. T. K. Ghanty, Former, Director, BSG)					
IL-13	Prof. Pradipta Bandyopadhyay, JNU, Delhi (Fast calculation of hydration free energy with both pure physics and physics based machine learning methods)	:			11:25-11:50hrs
IL-14	Prof. Abhijit Chatterjee, IIT, Bombay, Mumbai (Emergent ionic conduction in aliovalently-doped fast ion conductors)	:			11:50-12:15hrs
IL-15	Prof. Debashree Ghosh, IACS, Kolkata (Mechanism of Singlet fission in carotenoids)	:			12:15-12:40hrs
IL-16	Prof. Ateeque Malani, IITB, Mumbai	:			12:40-13:05hrs

	(Computational Design and Analysis of Porous Materials For Gas Separation and Storage)				
Lunch break: 13:00-14:00hrs					
Session-VII (14:00-15:55hrs)					
Parallel-A (main) (Dr. M. Deshpande, Head, ChTD)			Parallel-B (mini) (Dr. Nandini Garg, Head, MDS)		
IL-17	Prof. Rajesh Upadhyay, IIT BHU (DDPM Simulations of Liquid-Solids Binary Fluidized Bed and Validation via Radioactive Particle Tracking)	14:00-14:25 hrs	IL-20	Prof. Aftab Alam, IITB, Mumbai (Competing magnetic phases in the Weyl semimetal EuAuSb)	14:00-14:25 hrs
IL-18	Shri P. K. Sharma, BARC, Mumbai (Nuclear Fire Safety with Emphasis on CFD and Inclusion of Machine Learning)	14:25-14:50 hrs	IL-21	Dr. C. Majumder, BARC, Mumbai (Modeling Energy-Materials Using Density Functional Theory)	14:25-14:50 hrs
IL-19	Dr. K. K. Singh, BARC, Mumbai (Understanding flow physics in solvent extraction equipment using Computational Fluid Dynamics)	14:50-15:15 hrs	IL-22	Dr. M. K. Samal, BARC, Mumbai (A multiscale material model for simulation of high temperature deformation behavior of Nickel based superalloys)	14:50-15:15 hrs
ISL-13	Dr. K. C. Sandeep, BARC, Mumbai (Experimental and theoretical studies on the recovery of hydrogen isotopes from helium)	15:15-15:35 hrs	IL-23	Prof. Anil Kumar, NISER, Bhubaneswar (Nonreciprocal Interactions in active Systems)	15:15-15:40 hrs
ISL-14	Dr. Durga Prasad, BARC, Mumbai (A Multiscale Methodology to Determine Mechanical Properties of Irradiated Zirconium Alloys)	15:35-15:55 hrs	ISL-15	Dr. Srimanta Pakhira, IIT, Indore (Efficient Electrocatalytic H ₂ Evolution Mediated by 2D Transition Metal Dichalcogenides)	15:40-16:00 hrs
Tea Break: 16:00-16:25hrs					
Session-VIII (16:30-18:30hrs) (Chairs: Dr. P. Modak, Dr. K. Dasgupta, Dr. Rajesh Kumar, Dr. Durga Prasad, Dr. M. Chatterjee, Dr. B. Chakraborty, Dr. M. S. Shah, Dr. A. Boda, Dr. Arya Das, Dr. P. Sahu, Dr. D. Bandyopadhyay, Dr. A. K. Singha Deb)					
Poster presentation by participants (Abstract nos.: DAE-SAACM-A-2,A-3, A-5, A-6, A-7, B-1, C-1, C-3, C-4, C-5, C-7, C-8, C-9, D-5, D-7, D-8, E-3, E-4, E-5, E-7, F-3, F-4, F-5, F-6, F-7, F-8, F-11, F-12, F-14, F-15, F-16, F-18, G-3, G-4, G-5, G-6, H-2, H-3, H-4, H-5, I-2, I-6, I-7, O-18)				:	16:30-18:30hrs

Dinner (20:00-22:00hrs) at TSH

Day 3 (25 October, Friday, 2024)

**Session-IX (main) (09:30-11:00hrs)
(Chair: Dr. R. Tewari, Director, MG, BARC)**

PL-4	Dr. G. Sugilal, BARC, Mumbai (Numerical Study of Chaotic Mixing in Glass Melt Flows)	:	09:30-10:00hrs
PL-5	Prof. J. K. Singh, IIT, Kanpur (Digital Innovation for Accelerated Material Discovery: Integrating AI/ML and Molecular Simulations)	:	10:00-10:30hrs
IL-24	Prof. Jhumpa Adhikari, IITB, Mumbai (Molecular Insights into Liquid-Liquid Equilibria Obtained on Use of Alcohols for Efficient Extraction of Acetonitrile from Its Mixtures with Water)	:	10:30-10:55hrs

Tea break (10:55-11:25hrs)

Session-X (11:30-13:00hrs)

Parallel –A (main) (Chair: Dr. S. Mukhopadhyay, Head, ChED)			Parallel-B (mini) (Chair: Dr. A. Arya, Head, GAMD)		
IL-25	Dr. V. S. Phanikanth, BARC, Mumbai (Soil Structure Interaction Analysis of a Raft Foundation Supporting RC Chimney)	11:30-11:55 hrs	IL-27	Dr. P. Modak, BARC, Mumbai (Pressure Induced Insulator-to-Metal transition in TiS ₃)	11:30-11:55 hrs
IL-26	Dr. Prasannan Majumdar, BARC, Mumbai (Synthesis of multi-physics code PRABHAVINI for design and accident analysis of reactor system)	11:55-12:20 hrs	IL-28	Prof. Sushanta Mohapatra, CUH, Hyderabad (Conical Intersections and Quantum Chemical Dynamics)	11:55-12:20 hrs
ISL-16	Dr. Soumyadip Sett, IIT, Gandhinagar (Modeling Heat Transfer in Condensate Droplets during Dropwise Condensation)	12:20-12:40 hrs	IL-29	Dr. Sharat Chandra, IGCAR, Kalpakkam (Medium Range Order in Iron Phosphate Glasses)	12:20-12:45 hrs
ISL-17	Dr. Anurag Tripathi, IIT, Kanpur (Continuum simulation of granular flows in Rotating	12:40-13:00 hrs	ISL-18	Dr. Prateek Jha, IIT, Roorkee (Study of Light-Induced Self-Assembly of Functionalized	12:45-13:05 hrs

	cylinder and Orifice flows through rectangular hopper)			Nanoparticles using Quantum-Chemistry Derived Empirical Potentials)	
Lunch break: 13:00-14:00hrs					
Session-XI (14:00-16:00hrs)					
Parallel-A (main) (Chair: Shri K. Bhanja, Head, HWD)			Parallel-B (mini) (Chair: Dr. Arup Pathak, ChD, BARC & Dr. D. Bhandary, IIT, (BHU) Varanasi)		
ISL-19	Dr. Suneel Gattu, BARC, Mumbai (CFD based vitrification modelling during the Operational life cycle of Joule Heated Ceramic Melter – An Industrial application)	14:00-14:20 hrs	Oral presentation (12x10 minutes=2hrs) (Abstract no.: DAE-SAACM-A-4, A-8, B-2, C-10, D-9, E-1, E-2, F-9, F-13, G-1, G-2, J-1)		
ISL-20	Dr. Debashis Kundu, ICT, Jalna, (A Building Package for Crosslinked Polymer Structure)	14:20-14:40 hrs			
ISL-21	Dr. Nirvik Sen, BARC, Mumbai (Flow synthesis of ionic liquid in microreactors: Experiments, mathematical modelling and CFD modelling)	14:40-15:00 hrs			
ISL-22	Dr. Anoop Kishore, MIT, Bangalore (Ionic Liquids and Deep Eutectic Solvents as Asphaltene Aggregation Inhibitors: A Molecular Dynamics Simulations Study)	15:00-15:20 hrs			
ISL-23	Dr. Sourav Sarkar, BARC, Mumbai (The Droplet's Odyssey: A Computational Journey to Estimate Drag, Shape and Mass Transfer for a Drop)	15:20-15:40 hrs			
Tea break (16:00-16:30hrs)					
Session-XII (16:30-18:30hrs) (Chairs: Dr. P. Modak, Dr. K. Dasgupta, Dr. Rajesh Kumar, Dr. Durga Prasad, Dr. M. Chatterjee, Dr. B. Chakraborty, Dr. M. S. Shah, Dr. A. Boda, Dr. Arya Das, Dr. P. Sahu, Dr. D. Bandyopadhyay, Dr. A. K. Singha Deb)					
Poster presentation by participants (Abstract nos.: DAE-SAACM-K-1, K-3, K-4, L-4, L-5, M-3, M-4, M-8, M-10, M-11, M-12, M-13, M-15, N-2, N-3, O-5, O-6, O-8, O-13, O-14, O-15, O-17, O-20, O-21, O-22, O-23, O-24, O-25, O-26, O-27, O-28, O-29, O-30, O-31, O-33, O-34, P-1, P-3, P-6, P-7, P-8, P-9, A-9)				:	16:30-18:30hrs

Tea break (18:00-18:30hrs)			
SACM GB meeting (18:30-19:30hrs)			
Dinner (20:00-22:00) at DAE-CC			
Day 4 (26 October, Saturday, 2024)			
Session-XIII (main) (09:30-10:45hrs) (Chair: Dr. D. V. Udupa, Head, A&MPD)			
PL-6	Prof. A. K. Pati, TCG Crest, Kolkata (Quantum Speed Limit for Observables and Charging of Quantum Battery)	:	09:30-10:00hrs
IL-31	Dr. P. Shukla, BARC, Mumbai (Ingredients of Quantum Computing Technology at Superconducting Platform)	:	10:00-10:25hrs
ISL-24	Dr. Rahul Maitra, IITB, Mumbai (Molecular Energetics in Noisy Quantum Computers: Dynamic Construction of Ansatz via Operator Commutativity Screening to Avoid Local Traps and Barren Plateaus)	:	10:25-10:45hrs
Tea break (10:45-11:10hrs)			
Session-XIV (main) (11:15-13:00hrs) (Chair: Prof. A. K. Tyagi, Dean, HBNI)			
PL-7	Prof. B. Bagchi, IISc, Bangalore (Multidimensional Non Markovian Rate Theory With Applications to Diffusion and Nucleation)	:	11:15-11:45hrs
PL-8	Prof. G. N. Sastry, IIT, Hyderabad (Exploration of molecular interactions and chemical space: property-based classification using machine learning approaches)	:	11:45-12:15hrs
IL-32	Prof. R. Chakrabarti, IITB, Mumbai (Dynamics of active linear and ring polymers in porous media)	:	12:15-12:40hrs
IL-33	Dr. C. N. Patra, BARC, Mumbai (Polymers at interfaces: A Monte Carlo Density Functional Theory)	:	12:40-13:05hrs
Lunch break (13:00-14:00hrs)			
Session-XV (14:00-16:10hrs)			
Parallel-A (main) (Chair: Dr. R. Acharya, Head, IRAD)			Parallel-B (mini) (Chair: Dr. S. Mitra, SSPD)
IL-34	Dr. Rajeev Kapoor, BARC, Mumbai (Strength and ductility enhancement of hierarchically twinned Zr produced through multi-axial cryo-forging)	14:00-14:25 hrs	Oral presentation (13x10 minutes=2hrs 10min) (Abstract no.: DAE-SAACM-I-3, I-4, I-8, K-2, L-6, M-5, M-6, M-9, O-7, O-9, O-10, O-16, O-32)
IL-35	Dr. R. Mittal, BARC, Mumbai (Thermodynamic Behaviour of Novel Compounds: Neutron Scattering Experiments and Ab-initio Simulations)	14:25-14:50 hrs	
IL-36	Dr. Kinshuk Dasgupta, BARC, Mumbai (Carbon for Indian Atomic Energy Program)	14:50-15:15 hrs	

ISL-25	Dr. Sandip Khan, IIT, Patna (Interfacial Behavior of Aqueous Deep Eutectic Solvents and its application)	15:15-15:35 hrs	
ISL-26	Dr. Nafees Ahmed, BARC, Mumbai (Kinetic modeling and experimentation of Bunsen reaction in iodine-sulfur thermochemical process for production of hydrogen)	15:35-15:55 hrs	
Tea break (16:10-16:30hrs)			
Session-XVI (main) (16:30-17:30hrs) (Chair: K. T. Shenoy, Director, ChEG)			
Feedback and Concluding session			
Vote of Thanks: Dr. K. K. Singh, Secretary, DAE-SAACM2024			

- PL** : **Plenary Lecture**
EIL : **Emerging Investigator Lecture**
IL : **Invited Lecture**
ISL : **Invited Short Lecture**
main : **Main auditorium**
mini : **Mini auditorium**