JNCASR

ADVANCED QUANTUM THEORY 25 YEARS 2000 – 2025 MOLECULES TO MATERIALS

Frontiers in Multiscale Modeling of Molecules, Materials and Bio-materials

02 – 04 January, 2026

JNCASR, Bengaluru

Anusandhan National Research Foundation

Netweb TECHNOLOGIES

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Conference Schedule

Friday, January 02, 2026

12:00 – 14:00	Registration + Lunch
14:20 – 14:30	Opening Ceremony

Session 1
Chair: Sharma S. R. K. C. Yamijala

14:30 – 14:50	**Ayan Datta** *Buckling and Defects in Two-Dimensional Atomically Thin Monolayers*
14:50 – 15:10	**Anita Gemmy Francis** *High Pressure Tuning of Topological Phases in $TaSe_3$*
15:10 – 15:30	**Shubhajit Das** *Accelerating Catalyst Discovery in Challenging Chemical Spaces*
15:30 – 15:50	**Dibyajyoti Ghosh** *Atomistic and Machine Learning Guided Design of Dion-Jacobson Perovskites for High-Performance Optoelectronics*
15:50 – 16:20	***Group Photo + Coffee break***

Session 2
Chair: Sudipta Dutta

16:20 – 16:40	**Prakash Parida** *Light-Driven Two-dimensional Quantum Systems*
16:40 – 17:00	**Abhiroop Lahiri** *Attention-Based Kolmogorov-Arnold Networks as Variational Ansatze for Frustrated Quantum Spin Systems*
17:00 – 17:20	**Supriti Dutta** *Unravelling the Methanol Oxidation Mechanism over a Titania-Supported Platinum catalyst*
17:20 – 17:30	**Utkarsh Singh** *Organic Scaffolds for Tunable Triplet Emission: A Computational Perspective*
19:00	***Dinner***

Saturday, January 03, 2026

Session 3 **Chair: Arun K Manna**	
9:30 – 9:50	**Bradraj Pandey** *Dynamics, Fusion, and Braiding of Majorana Zero Modes in Quantum Dot–Based Interacting Kitaev Chains*
9:50 – 10:10	**Sasmita Mohakud** *Realization of Altermagnetism by Structural Engineering*
10:10 – 10:30	**Sairam S. Mallajosyula** *Refinement of the Drude Polarizable Force Field for Hexose Monosaccharides: Capturing Ring Conformational Dynamics with Enhanced Accuracy*
10:30 – 10:40	**Pralhad Shenoy** *Computational Investigations into the Mechanisms of $Mn(aNHC)Br(CO)_4$ Catalyzed Aldehyde Reduction*
10:40 – 11:00	***Coffee break***

Session 4 **Chair: Ayan Datta**	
11:00 – 11:20	**Sudipta Dutta** *Designing Two-Dimensional Noncentrosymmetric Systems for Valley-Polarization*
11:20 – 11:40	**Suparna Sarkar** *Flux Driven Circular Current and Localization Transition in non-Hermitian Systems*
11:40 – 12:00	**Pralok K Samanta** *Modelling of Excited State Properties in Narrow-Band Organic Emitters*
12:00 – 12:20	**Swastika Banerjee** *Computational Insights into Super-Ionic Conductors for Next-Generation Solid-State Batteries*

12:20 – 12:30	**Sayan Paul** *Unusual Particle-to-Wave Phonon Crossover Leads to Ultralow Lattice Thermal Conductivity in Tl_2AgI_3*
12:30 – 14:30	***Lunch break***

Session 5 **Chair: Lakshmi Sankaran**	
14:30 – 14:50	**Pallavi Sarkar** *Organic Photoredox Catalysis for CO_2 Reduction*
14:50 – 15:10	**Raju K Biswas** *Emergence of ultra-low lattice thermal conductivity and high thermo-electric performance in chiral phonon-protected heterostructures*
15:10 – 15:30	**Arkamita Bandyopadhyay** *Topology-Driven Quantum Toroidal Moments in N-Doped Carbon Nanotori for Next-Generation Qubit Design*
15:30 – 15:50	**Vipin Raj K** *Synergistic Effects of Surface Defects and Donors in Stereoselective Ziegler-Natta Catalysis: An Ab Initio Study*
15:50 – 16:20	***Coffee break***

Session 6 **Chair: Prakash Parida**	
16:20 – 16:40	**Bidhan Chandra Garain** *Unsupervised Learning for Excited-State Pathways*
16:40 – 17:00	**Madhulika Mazumder** *Navigating Structural Complexities and Redox Mechanisms in Li Rich Layered and Spinel Oxide Cathode Materials*
17:00 – 17:10	**Soumya Satpathi** *Phases and Phase Transitions in 1D Alternating Spin ($\frac{1}{2}$, 1) Chain: Effects of Frustration and Anisotropy*
17:30 –19:30	Cultural program
19:30	***Dinner***

Sunday, January 04, 2026

Session 7
Chair: Sairam S. Mallajosyula

9:30 – 9:50	**Neha Bothra** *Synergistic Coupling of Anionic Oxygen Redox with Selenium for Stable High-voltage Sodium Layered Oxide Cathodes*
9:50 – 10:10	**Sharma S. R. K. C. Yamijala** *Plasmon-Induced Hot Carriers: Generation, Dynamics, and Environmental Applications*
10:10 – 10:20	**Mayank Sharma** *Elucidating Thermodynamic Infeasibility of (De)-Lithiation Process in 5V-class $LiNi_{0.5}Ge_{1.5}O_4$ Solid Electrolyte*
10:20 – 10:30	**Sougata Saha** *Computational Modeling of Metal Doped Carbon Nanostructures for Electrochemical Water Splitting and Metal Air Battery Applications*
10:30 – 11:00	***Coffee break***

Session 8
Chair: Dibyajyoti Ghosh

11:00 – 11:20	**Arun K Manna** *Computational Insights into the Molecular Photophysics: Toward Triplet Photosensitization*
11:20 – 11:40	**Supriya Ghosal** *Quaternary Half-Heusler: A Potential Platform to Suppress Lattice Thermal Conductivity Towards Improved Thermoelectric Performance*
11:40 – 12:00	**Somananda Sanyal** *Beyond Academia: Exploring career growth in academic publishing industries Evolution*
12:00 – 12:20	**Swapan K Pati** *Modeling Electronics in Nanomaterials and Frustration in Physics and Chemistry*

12:20 – 1:00	Conclusion & vote of thanks
1:00	***Lunch***