

PHYSICS AND CHEMISTRY OF ATOMIC, MOLECULAR AND CONDENSED MATTER SYSTEMS (PCAMC - 2024)

DECEMBER 11, 2024 (WEDNESDAY)

REGISTRATION (02:00 - 04:00 PM) and High Tea 3:30- 4:00 PM

INAUGURAL PROGRAM (04:00 - 04:15 PM)

	Chairperson: Amlan K. Roy, IISER Kolkata
04:15-04:45	Debashis Mukherjee (CQuERE TCG CREST) <i>Aspects of correlation in the many-electron problem.</i>
04:45-05:05	P. Balanarayan (IISER Mohali) <i>Harmonic Generation Spectra from Argon atoms with time delayed IR Pulse</i>
05:05-05:35	Peter Saalfrank (University of Potsdam) <i>Correlated wavefunction approaches to laser-driven electron dynamics in molecules and their control.</i>

TEA/COFFEE (05:35 – 05:45 PM)

	Chairperson: Debasis Koley, IISER Kolkata
05:45-06:15	V. Subramanian (IIT Madras) <i>Development of Small Organic Molecules with TADF Activity.</i>
06:15-06:35	C.N. Ramachandran (IIT Roorkee) <i>Formation of Gas Hydrates: A Computational Approach</i>
06:35-06:55	Mudit Dixit (CLRI Chennai) <i>Accelerating Materials Discovery for Catalysis and Electrochemical Energy Storage.</i>

DINNER (7:30 PM onwards)

DECEMBER 12, 2024 (THURSDAY)

	Chairperson: Mousumi Das, IISER Kolkata
09:30-10:00	N. Sathyamurthy (IISER Mohali) <i>Anions in interstellar media.</i>
10:00-10:30	Sanjay Kumar (IIT Madras) <i>Ab Initio Bound-State Structural and Quantum Dynamics Studies of Charge-Transfer Processes in Ion-Molecule Collisions at High (keV) Collision Energies relevant to Cometary Environments</i>
10:30-10:50	Manikandan Paranjothy (IIT Jodhpur) <i>Classical Trajectory Simulations of $CN^- + CH_3I$ Bimolecular Nucleophilic Substitution Reaction.</i>

TEA/COFFEE (10:50 – 11:10 AM)

	Chairperson: Susmita Roy, IISER Kolkata
11:10-11:40	Santanu Bhattacharya (IISER Tirupati) <i>On the Role of Chirality in Self-Organizing Systems.</i>
11:40-12:00	Hridyesh Mishra (Banaras Hindu University) <i>Dynamics of Fluorescence Quenching and Stabilization of enol-keto Structures of the Salicylate Anion in Acetonitrile and Water.</i>
12:00-12:20	Ankan Paul (IACS Kolkata) <i>Comprehending Toluene Oxidation to Benzaldehyde through Photoinduced Host Guest Electron Transfer and Ultrafast C–H Bond Activation.</i>
12:20-12:40	Manabendra Sarma (IIT Guwahati) <i>Insights into Photodynamics Simulation of Excited-State Relaxation Mechanism of GFP Chromophore and its Derivatives</i>
12:40-01:00	Kshatresh Dutta Dubey (Shiv Nadar University) <i>Designing Catalysts based on Designed Local Electric Field.</i>
LUNCH BREAK (01:00 – 02:00 PM)	
	Chairperson: T. Rajagopala Rao, IIT Patna
02:00-02:30	Satrajit Adhikari (IACS Kolkata) <i>The effect of surface temperature on the chemisorption: A benchmark collision process with H_2/D_2 – Cu(111) system.</i>
02:30-02:50	Upakarasamy Louderaj (NISER Bhubaneswar) <i>Mechanisms and Dynamics of Bimolecular Nucleophilic Substitution Reactions.</i>
02:50-03:10	Brijesh Mishra (Krea University) <i>The effect of confinement on PH_3 and OH_3^+ inversion inside C_{60}</i>
03:10-03:30	Amit Kumar Paul (Bose Institute Kolkata) <i>Dynamics of Aromatic Complexes at High Temperatures.</i>
03:30-03:50	Padmabati Mandal (IISER Tirupati) <i>Non-adiabatic Photodissociation Dynamics of Indole using Multi-Configuration Time-dependent Hartree Method.</i>
TEA/COFFEE (03:50 – 04:10 PM)	
	Chairperson: Ranganathan Subramanian, IIT Patna
04:10-04:40	Susanta Mahapatra (University of Hyderabad) <i>Quantum Dynamics of Chemical Systems of Astrophysical Interest</i>
04:40-05:00	Biswajit Maiti (Banaras Hindu University) <i>Role of spin crossover in the photodissociation dynamics.</i>
05:00-05:20	T.J. Dhillip Kumar (IIT Ropar) <i>Rotational Transitions of Linear C_5 with H_2 Collision at Interstellar Temperatures.</i>

05:20-05:40	Sarvesh Kumar Pandey (MANIT Bhopal) <i>New Insights into Some Possible Formation Pathways of CH_3OCH_3 and CH_3SCH_3 in the Interstellar Medium and Potential Role of Alkali Metal-Ion Therein.</i>
05:40-06:00	Subhash Ghosal (NIT Durgapur) <i>Structure, Dynamics, and Spectroscopy of hydrocarbon molecules recently detected in the interstellar medium.</i>
POSTER SESSION (06:45 – 7:45 PM)	
DINNER (08:00 PM onwards)	
DECEMBER 13, 2024 (FRIDAY)	
	Chairperson: Goutam Dev Mukherjee, IISER Kolkata
09:30-10:00	Sourav Pal (Ashoka University) <i>Conceptual Density Functional Theory: Applications to Catalysis.</i>
10:00-10:30	Indra Dasgupta (IACS Kolkata) <i>Spin-orbit driven emergent phases in quantum materials.</i>
10:30-10:50	Rotti Srinivasamurthy Swathi (IISER Thiruvananthapuram) <i>Global Optimization of Atomic and Molecular Clusters Bound to Carbon Nanostructures: A Swarm Intelligence Approach.</i>
TEA/COFFEE (10:50 – 11:10 AM)	
	Chairperson: Neelanjana Sengupta, IISER Kolkata
11:10-11:40	Sundaram Balasubramanian (JNCASR Bangalore) <i>Learning Materials Science through Machine-Learned Potentials.</i>
11:40-12:00	Vivek Kumar Yadav (University of Allahabad) <i>Energy and Environmental Applications through Doping in 2D Fullerene Networks</i>
12:00-12:20	Hemant Kumar Kashyap (IIT Delhi) <i>Mechanism of Solid-Electrolyte Interphase (SEI) Formation Near Lithium Metal Surface.</i>
12:20-12:40	Rajarshi Chakrabarti (IIT Bombay) <i>Dynamics of active tracer particles in complex environments: insights from computer simulations.</i>
12:40-01:00	Arnab Bhattacharjee (JNU) <i>Uncovering High-Resolution Organization of Genomic Loci via Multiscale Polymer Simulations</i>
LUNCH BREAK (01:00 – 02:00 PM)	
	Chairperson: K. Balamurugan, CLRI Chennai
02:00-02:30	Tanusri Saha Dasgupta (SNBNCBS Kolkata) <i>Machine Learning Approach of Design of New Materials with Targeted Properties</i>
02:30-02:50	Subhasish Sinha (IISER Kolkata) <i>Chaos and emergence of a quasi-ergodic steady state in a dissipative Tavis-Cummings array.</i>

02:50-03:10	Manoranjan Kumar (SNBNCBS Kolkata) <i>Quantum Phases in Coupled Trimer Materials.</i>
03:10-03:30	Sourin Das (IISER Kolkata) <i>Majorana bound state and odd-frequency superconducting pairing in 2-D topological insulator.</i>
03:30-03:50	Siddhartha Lal (IISER Kolkata) <i>New insights on metal-Mott insulator transitions.</i>
TEA/COFFEE (03:50 – 04:10 PM)	
	Chairperson: Jyotirmayee Dash, IACS Kolkata
04:10-04:40	Sushanta Dattagupta (Sister Nivedita University Kolkata) <i>Rashba effect in angle-resolved magneto resistance in a 2- dimensional oxide layer.</i>
04:40-05:00	Tulika Maitra (IIT Roorkee) <i>Emerging triferroicity and polar metallic state in two dimensional rare-earth halide based monolayers.</i>
05:00-05:20	Shivnath Majumder (IIT Jammu) <i>AI-Driven Discovery of Asymmetric Pauson-Khand Reactions: A New Toolbox in a Synthetic Chemist's Treasure</i>
POSTER SESSION (05:20 – 07:00 PM)	
BANQUET DINNER (7:30 PM)	
DECEMBER 14, 2024 (SATURDAY)	
	Chairperson: Gaurav Shukla, IISER Kolkata
09:00-09:20	Ayan Datta (IACS Kolkata) <i>Buckling and Defects in Two - Dimensional Atomically Thin Monolayers.</i>
09:20-09:40	Sai G. Ramesh (IISc Bangalore) <i>Nuclear Quantum Effects in Gas-Phase 2X-Ethanols</i>
09:40-10:00	Vidya Avasare (Ashoka University) <i>Origin of Selectivity in the Gold Catalyzed Aminoauration of Alkynes.</i>
10:00-10:20	Mehboob Alam (IIT Bhilai) <i>Theoretical design of photosensitizers for photodynamic therapy applications</i>
10:20-10:40	Pradeep Kumar (MNIT Jaipur) <i>Impact of Water on Lifetime of HO₃ radical in the Atmosphere: Role of Non-Statistical Effects</i>
10:40-11:00	Saurabh Srivastava (Manipal University Jaipur) <i>A Train of Single Molecule-Gears on Surface: Computational Approach</i>

TEA/COFFEE (11:00 – 11:20 AM)	
	Chairperson: Swastika Chaterjee, IISER Kolkata
11:20-11:40	Rahul Maitra (IIT Bombay) <i>Projective Quantum Eigensolver with Generalized Operators: a Noise-resilient Algorithm for Noisy Quantum Hardware</i>
11:40-12:00	Amber Jain (IIT Bombay) <i>Energy transfer in molecular wires: new insights</i>
12:00-12:20	Soumya Mukherjee (MANIT Bhopal) <i>Introduction of Complex Diabatization Technique: Formulation and Applications.</i>
12:20-12:40	Bijit Mukherjee (University of Warsaw) <i>Towards a sample of stable ultracold molecular gas.</i>
12:40-01:10	Trygve Helgaker (University of Oslo) <i>Molecular Dynamics and Rovibrational Spectra in a Magnetic Field.</i>
CONCLUDING REMARKS (01:10 PM)	
LUNCH (01:30 PM onwards)	