

DAY 1 - Monday , 05/10/2026

Poster Board No.	Name	Abstract ID	Title	Category
1	Ms. Priyanka Yadav	ICMS2026-A-2	<u>Folding Pathways and Force-Induced Unfolding of Neurodegeneration Associated GGGGCC Microsatellite Repeat RNA Revealed by Molecular Simulations</u>	Biological Systems and Medicine
2	Dr. Avijeet Kulshrestha	ICMS2026-A-3	<u>The transmembrane domain regulates the kinetics of the SARS-CoV-2 spike conformational transition</u>	Biological Systems and Medicine
3	Ms. Aysha Fahmeetha	ICMS2026-A-4	<u>Structural Dynamics of a small GTPase implicated in Huntington's Disease</u>	Biological Systems and Medicine
4	Ms. Surabhi Singh	ICMS2026-A-6	<u>Beyond Sequence: Integrating Molecular Dynamics, DNA Shape, and Binding Energetics to Understand Protein-DNA Binding</u>	Biological Systems and Medicine
5	Ms. Anshika Tiwari	ICMS2026-A-9	<u>Atomic-Level Insights into the Adsorption on Boron Nitride Nanosheets for Wastewater Treatment Applications</u>	Biological Systems and Medicine
6	Mr. SOUMYA ROY	ICMS2026-A-11	<u>Microscopic Insights into Osmolyte Effects on the Solvation Shell Structure and Dynamics around a Protein in Aqueous Medium</u>	Biological Systems and Medicine
7	Mr. PRATYUSH PANI	ICMS2026-A-12	<u>Decoding the Allosteric Regulatory Landscape of Brain-Specific Kinase 2 (BRSK2) Using Multi-Scale Molecular Dynamics and Temporal Graph Neural Networks</u>	Biological Systems and Medicine
8	Dr. Chandramouli Natarajan	ICMS2026-A-19	<u>REHT-PMP: an efficient sampling method for capturing the conformational changes of peripheral membrane proteins on lipid bilayers</u>	Biological Systems and Medicine
9	Ms. Vinodhini Selvanarayanan	ICMS2026-A-22	<u>Evolutionary differences affecting conformational selection of EHD paralogs: insights from molecular simulations and implications in membrane remodeling.</u>	Biological Systems and Medicine
10	Mr. Arkadeep Banerjee	ICMS2026-A-23	<u>Understanding How Self-Peptides Modify Protein Folding</u>	Biological Systems and Medicine
11	Mr. Akshay Chauhan	ICMS2026-A-25	<u>Sequence Architecture Governs Condensate Nucleation While Condensate Size Controls Protein Specialization in Multicomponent Chromatin</u>	Biological Systems and Medicine
12	Mr. sankalp Jadhav	ICMS2026-A-29	<u>The GYG Interface as the Missing Ice-Nucleating Site: Why Dimerization Is Required for Class C Bacterial Ice Nucleation</u>	Biological Systems and Medicine
13	Ms. Aakanksha Kunwar	ICMS2026-A-30	<u>Revealing the Binding and Drug resistance mechanism of Doravirine complexed with Wild-type and Mutant HIV-1 Reverse Transcriptase using Multiple-Molecular Dynamics Simulation</u>	Biological Systems and Medicine
14	Ms. Jessica Baa	ICMS2026-A-33	<u>Characterizing the nanoscale dynamics and differential binding of Tropomodulin and Leiomodin with actin filaments</u>	Biological Systems and Medicine
15	Mr. RISHAV DEB	ICMS2026-A-36	<u>Determining effect of point mutations on HIV-1 VpX-SAMHD1 interaction. using MD simulation approach</u>	Biological Systems and Medicine
16	Ms. Richa Shetty	ICMS2026-A-37	<u>Molecular Dynamics Elucidation of Nanoplastic Induced Neurotoxicity via CNS GPCR Interactions</u>	Biological Systems and Medicine
17	Ms. Shikha Kumari	ICMS2026-A-38	<u>Electrospun Castor Oil-Derived Polyurethane with PHA and Chitosan Composite Nanofibers for Biodegradable Wound Dressing Applications</u>	Biological Systems and Medicine
18	Dr. Manas Sharma	ICMS2026-B-1	<u>From Molecules To 2D Magnets: ML-Driven Insights into CrCl3 (2D MM) Synthesis</u>	Catalysis and Surface Science
19	Mr. Jogeswar Chhatria	ICMS2026-B-5	<u>Overcoming Interfacial Kinetic Barriers in 5- Hydroxymethylfurfural Extraction Using Salt and Amphiphilic Modifiers in Water-Supercritical CO2 Biphasic Systems</u>	Catalysis and Surface Science
20	Mr. SAIKAT SAHA	ICMS2026-B-6	<u>Comparative Assessment of Exchange–Correlation Functionals in Furfural Surface and Reaction Modeling</u>	Catalysis and Surface Science
21	Mr. Prakyath Thalya	ICMS2026-B-9	<u>Rational Design of Transition Metal catalysts for methane activation using DFT-ML</u>	Catalysis and Surface Science
22	Mr. Neil Shanmukh Nanduri	ICMS2026-B-11	<u>Investigation and design of augmented theozymes for superior control of de novo enzyme active sites</u>	Catalysis and Surface Science
23	Mr. Subhajit Pat	ICMS2026-B-14	<u>Molybdenum Catalyst and Peroxide based Enantiomeric Epoxidation of Allylic Alcohols: Probing Selectivity & Suppressed Racemization via DFT Calculations</u>	Catalysis and Surface Science
24	Mr. Sougata Saha	ICMS2026-B-16	<u>Modeling of Metal Doped Carbon Nanostructures for Electrochemical Water Splitting and Metal Air Battery Applications</u>	Catalysis and Surface Science
25	Dr. Aditya Goyal	ICMS2026-B-32	<u>Descriptor-Based Screening of Metal Chloride Dopants for Methane Activation in Molten KCl</u>	Catalysis and Surface Science
26	Mr. Bharath Desikan	ICMS2026-F-16	<u>Altering interfacial thermodynamics of methanol-water solutions using Angstrom-scale graphene nanopores for enhanced evaporative separations</u>	Catalysis and Surface Science
27	Mr. Sree Bharadwaj H	ICMS2026-B-31	<u>Multi-fidelity computational screening of high-entropy MBenes for electrochemical CO2 reduction</u>	Catalysis and Surface Science
28	Dr. Sagar Chandra	ICMS2026-C-1	<u>Atomistic Modeling of Interface Mediated Deformation and Twin Nucleation in Ni-Based Superalloys</u>	Computational Material Sciences

29	Mr. SANKHASUBHRA MUKHOPADHYAY	ICMS2026-C-2	<u>Investigation of Phase Stability and Diffusional Aspects for Rhodium-Barium Alloy System Using a Developed Embedded-Atom Method Potential</u>	Computational Material Sciences
30	Mr. Prehas Madke	ICMS2026-C-3	<u>A DFT Study of Experimentally Guided Biochar Structure for CO₂ Adsorption: The Role of Surface Functional Groups</u>	Computational Material Sciences
31	Mr. Madhurja Buragohain	ICMS2026-C-6	<u>Unveiling the Role of Ion Pairs in Determining Electrolyte Stability and Solid Electrolyte Interphase Formation in Lithium Metal Batteries</u>	Computational Material Sciences
32	Mr. Debendra Meher	ICMS2026-C-7	<u>Superionic boron diffusion in dense crystalline B₂O₃</u>	Computational Material Sciences
33	Dr. Soumya Mishra	ICMS2026-C-8	<u>Dislocation Pinning by Vacancy Loops in Irradiated Tungsten: A Molecular Dynamics Study</u>	Computational Material Sciences
34	Ms. CHARITHA DODDI	ICMS2026-C-13	<u>Quantifying the Structural Stability of C15-like Defect Clusters and Their Interactions with Point Defects in Irradiated Tungsten</u>	Computational Material Sciences
35	Mr. Yuki Kitamura	ICMS2026-C-14	<u>Atomistic Insights into Localization and Diffusion of Water Molecules in Edible Oils</u>	Computational Material Sciences
36	Mr. Soumyadeep Chowdhury	ICMS2026-C-15	<u>Molecular Insights into Crosslinking Architecture in Sulfur-Vulcanized Elastomers</u>	Computational Material Sciences
37	Ms. Antaripa Saha	ICMS2026-C-18	<u>An Atomistic study of high-pressure Reverse Osmosis for the separation of NaNO₃ through a polymeric membrane: A Non-Equilibrium Molecular Dynamics Simulation (NEMD)</u>	Computational Material Sciences
38	Ms. Yati Sharma	ICMS2026-C-19	<u>Atomistic Design Principles for Enhanced Lithium-Ion Conduction in Solid-State Electrolytes</u>	Computational Material Sciences
39	Dr. Avinash Chauhan	ICMS2026-C-21	<u>Self-Organization Dynamics in a One Component Active Matter System</u>	Computational Material Sciences
40	Mr. Mohammad Awwab Saiyad	ICMS2026-C-22	<u>Novel High-Pressure Phases in La-Ta-H Ternary Hydrides and Investigation of Their Electronic and Superconducting Properties</u>	Computational Material Sciences
41	Ms. Manya Aggarwal	ICMS2026-C-24	<u>Uncovering the molecular origins of water organization and activity in organic solvent/water and water-in-salt electrolytes</u>	Computational Material Sciences
42	Mr. Nikhil Singh	ICMS2026-C-25	<u>Hot Carrier Relaxation in Halide Double Perovskites: Insights from Ab Initio Models and Structure-Informed Machine Learning</u>	Computational Material Sciences
43	Mr. Mohd Adnan	ICMS2026-C-26	<u>Understanding Adsorption of Asphaltene and Resin Molecules on Iron Oxide Surfaces: Molecular Simulation Study</u>	Computational Material Sciences
44	Mr. VAISHNAV RAVEENDRAN	ICMS2026-C-29	<u>Density Functional Theory Studies of KNiF₃-Based Perovskites and MXene Composites for Supercapacitor Applications</u>	Computational Material Sciences
45	Mr. Subhom Ghosh	ICMS2026-D-4	<u>MACE-GEN: A Generalized Score-Based Diffusion Framework for Amorphous Materials</u>	Machine Learning and AI, and Molecular Modeling
46	Mr. Satya Chaithanya Duggisetty	ICMS2026-D-5	<u>NBAR-mediated membrane deformations at multiples scales using integrated continuum mechanics and molecular simulations</u>	Machine Learning and AI, and Molecular Modeling
47	Dr. Anjali Rameja	ICMS2026-D-6	<u>DFT-accurate machine learning interatomic potential for Mg -Ca bulk metallic glasses: fine-tuning MACE-MP-0 and benchmarking against 2NN-MEAM</u>	Machine Learning and AI, and Molecular Modeling
48	Mr. Amar Yadav	ICMS2026-D-10	<u>Deep-learning Guided Sequence Design and Multiscale Molecular Characterization of Human VCP Double-Psi β-Barrel with Improved Biophysical Properties</u>	Machine Learning and AI, and Molecular Modeling
49	Mr. Nandu S	ICMS2026-D-11	<u>Fundamental Underpinnings of Ion-π Interactions: Essence and Nature</u>	Machine Learning and AI, and Molecular Modeling
50	Mr. Sai Athmeeya Shet	ICMS2026-D-12	<u>Development of a Machine Learning Interatomic Potential for Molecular Dynamics Simulations of PVC-Plasticizer Systems</u>	Machine Learning and AI, and Molecular Modeling
51	Mrs. Monika Angwani	ICMS2026-F-2	<u>Estimation of Transition Pathways and Free energies via Transition Matrix Monte Carlo</u>	Theory and Methodology
52	Mr. Rahul Sharma	ICMS2026-F-3	<u>Variational Adaptive Gaussian Decomposition: Scalable Quadrature-Free Time-Sliced Thawed Gaussian Dynamics</u>	Theory and Methodology
53	Mr. Vipin Kumar	ICMS2026-F-5	<u>Solubility Calculation of Glycine Polymorphs using Einstein Molecule Method</u>	Theory and Methodology
54	Dr. Dmitry Lesovoy	ICMS2026-F-6	<u>Conformational heterogeneity of proteins in silica - functional dynamics or prediction artefacts: solution NMR experimental validation in focus.</u>	Theory and Methodology
55	Mr. Shuvam Banerji Seal	ICMS2026-F-8	<u>Is KMAP Possible? Formal Verification of Karnaugh Map Encoding for Biological Sequences in Lean 4</u>	Theory and Methodology

56	Ms. Parvathi K	ICMS2026-G-1	<u>Entropy, Free Energy, and a Generalized Order Parameter for Liquid Crystal Phases of Chiral and Achiral Rods</u>	Polymers and Soft Matter
57	Dr. Tushar Mahendrakar	ICMS2026-G-3	<u>Free Energy Landscapes, Nucleation, and Morphological Stability of Biphasic Nanodroplets Dispersed in a Liquid Phase</u>	Polymers and Soft Matter
58	Mr. Pankaj Adhikary	ICMS2026-G-5	<u>Cross-Amine Bidentate Water: The Overlooked Origin of Rotational Slowdown in Aqueous Urea</u>	Polymers and Soft Matter
59	Ms. Minakshi Jangir	ICMS2026-G-7	<u>Activity-induced patterns in polymer-grafted active colloids</u>	Polymers and Soft Matter
60	Mr. Amartya Sam	ICMS2026-G-8	<u>Self-Assembly and Interfacial Behavior of Hairy Nanoparticles</u>	Polymers and Soft Matter
61	Mr. RAJ GAURAV	ICMS2026-G-9	<u>Comparative Study of Healthy and Diseased Red Blood Cells in Shear Flow</u>	Polymers and Soft Matter
62	Ms. Manasi Lavhekar	ICMS2026-D-79	<u>Optimization of 2D Nanopore Structures in Graphene for Gas Separation Using Artificial Intelligence</u>	Machine Learning and AI, and Molecular Modeling

DAY 2 - Tuesday, 06/10/2026

Poster Board No.	Name	Abstract ID	Title	Category
1	Ms. Nirupma Rani	ICMS2026-A-39	<u>Covalent Cross-Linking Enhances Thermal Robustness of Archaeal Tetraether Membranes: Insights from Molecular Dynamics Simulations</u>	Biological Systems and Medicine
2	Mr. Amar Krishna Gopinath	ICMS2026-A-40	<u>Fold, Flip, and Cross: How Chain Length Controls Surfactant Transport through Bacterial Outer Membrane Channels</u>	Biological Systems and Medicine
3	Dr. Digvijay Prakash	ICMS2026-A-42	<u>Investigating RNA-Guided Assembly of Phage Qβ Using Coarse-Grained Structure-Based Models</u>	Biological Systems and Medicine
4	Ms. ANJALIN JOY	ICMS2026-A-49	<u>The Essential Role of Base Catalysis in Flavin-Mediated Alcohol Oxidation</u>	Biological Systems and Medicine
5	Mr. Rithwik Nambiar	ICMS2026-A-50	<u>A Comparative Evaluation of Dimensionality Reduction Methods for Molecular Dynamics Simulations</u>	Biological Systems and Medicine
6	Mr. Naren C	ICMS2026-A-52	<u>Role of Monomer Folding Pathway in Domain Swapping of Monellin</u>	Biological Systems and Medicine
7	Mr. Nishant Bahuguna	ICMS2026-A-54	<u>Role of cardiolipin in CM15 binding in bacterial membranes</u>	Biological Systems and Medicine
8	Ms. Shahana C	ICMS2026-A-55	<u>Molecular Dynamics Investigation of the Self-Assembly of Aromatic Amino Acids: Phenylalanine, Tyrosine and Tryptophan</u>	Biological Systems and Medicine
9	Mr. Antony John	ICMS2026-A-56	<u>Comparison of single-pass transmembrane helix dynamics of Class I viral fusion protein and human fusion protein.</u>	Biological Systems and Medicine
10	Mr. Manoj B	ICMS2026-A-58	<u>Unraveling the molecular mechanism of temperature sensitivity in human TRPV1</u>	Biological Systems and Medicine
11	Ms. Khushboo Bhagat	ICMS2026-A-60	<u>Replica Exchange Molecular Dynamics and Experimental Validation Reveal Enhanced Thermostability of a Rationally Redesigned Primordial Double-Psi β-Barrel Domain</u>	Biological Systems and Medicine
12	Ms. Srishti Batra	ICMS2026-A-61	<u>ProChartS: A Label-Free, Non-Invasive Protein Spectroscopic Probe: pH/Temperature Sensitivity and ML-Accelerated Spectral Prediction</u>	Biological Systems and Medicine
13	Mr. Susanta Mandal	ICMS2026-A-62	<u>Kaempferol-Mediated Disruption of Aβ Protofibrils: Mechanistic Insights from Molecular Docking and Molecular Dynamics Simulation Study</u>	Biological Systems and Medicine
14	Ms. Kriti Shukla	ICMS2026-A-63	<u>Dynamics of Water Reorganization and Proton Transfer in Human Carbonic Anhydrases</u>	Biological Systems and Medicine
15	Ms. Sudipti Priyadarsinee	ICMS2026-A-64	<u>Conformation-dependent reactivity and unbinding dynamics of an inhibitor of ribonuclease A</u>	Biological Systems and Medicine
16	Mr. DULAL MONDAL	ICMS2026-A-65	<u>Conformation-Dependent Sidechain pKa from Constant pH and Two-Dimensional Replica Exchange MD Simulation in an Enzyme</u>	Biological Systems and Medicine
17	Mr. Ramesh Yadav Kanchugantla	ICMS2026-A-96	<u>Molecular simulations of Protein Translocation through Carbon Nanotubes reveal its conformational dynamics</u>	Biological Systems and Medicine
18	Mr. Swastik Laha	ICMS2026-C-30	<u>Facet-dependent oxygen evolution on IrO₂ from machine-learned potential-driven atomistic models</u>	Computational Material Sciences
19	Mr. Sanjib Ray	ICMS2026-C-32	<u>Investigation of Proton Transport Mechanism in Sc-doped CaZrO₃ using Ab-initio Molecular Dynamics Simulations</u>	Computational Material Sciences
20	Mr. Suman Bhadra	ICMS2026-C-33	<u>Deciphering Hidden Charge Transport Pathways in Break-Junction Conductance Histograms of TPTZ Molecular Breadboards</u>	Computational Material Sciences
21	Dr. ARKA PRAVA SARKAR	ICMS2026-C-35	<u>Investigating the nature of anion migration in halide perovskites in presence of single layer graphene</u>	Computational Material Sciences
22	Mr. Dhiman Hazra	ICMS2026-C-37	<u>Green-Kubo Approach to Thermal Conductivity Prediction in Tp-Based and Related Covalent Organic Frameworks (COFs)</u>	Computational Material Sciences
23	Mr. Puneet Kumar	ICMS2026-C-39	<u>Sodium Ion Diffusion Behavior in Na₃Si₆O₁₅ Solid-State Glass Electrolyte: Insights From ab initio Molecular Dynamics</u>	Computational Material Sciences
24	Ms. Afi J M	ICMS2026-C-41	<u>Thickness Dependent Dielectric Response of Confined Water</u>	Computational Material Sciences
25	Ms. Ramya Lakshmi	ICMS2026-C-42	<u>Atomistic Calculations of Vacancy Formation Energy in Concentrated Alloys</u>	Computational Material Sciences
26	Ms. Suchitra D	ICMS2026-C-45	<u>Atomistic Investigation of Hydrogen Diffusion, Segregation Energy, and Critical Resolved Shear Stress in Al-Mg-Zr Alloys for Type III Hydrogen Storage Tank Applications</u>	Computational Material Sciences
27	Ms. Mansi Jain	ICMS2026-C-46	<u>Molecular Origins of the Conductivity Difference Between DMC- and DEC-Based Electrolytes</u>	Computational Material Sciences
28	Ms. Pritichhanda Barik	ICMS2026-C-47	<u>Computational study of Metal Organic Frameworks for the adsorption and conversion of corrosive NO₂ to ammonia using molecular simulations</u>	Computational Material Sciences
29	Mr. KUMAR SHANU	ICMS2026-C-48	<u>Atomistic insights into free volume, barrier and rheological behavior of graphene - oxide reinforced PLA nanocomposites using MD simulations</u>	Computational Material Sciences
30	Mr. Sumitro Dey	ICMS2026-C-49	<u>Self Assembly and Microscopic Mechanical Properties of Small Molecule Modified DNA Hydrogels</u>	Computational Material Sciences
31	Mr. Srinibas Nandi	ICMS2026-C-54	<u>Efficient finite-element based DFT methods using meta-GGA functionals with accelerated self-consistent field iterations</u>	Computational Material Sciences
32	Mr. Subham Das	ICMS2026-C-55	<u>Understanding oxidation behaviour in dual-phase CoCrNiCu_{0.5} alloy: A combined experimental and theoretical study</u>	Computational Material Sciences
33	Mr. Sai Anirudh Guttapati	ICMS2026-C-58	<u>Finite-element Implementation of LDOS Preconditioner for Accelerated SCF Convergence in Density Functional Theory</u>	Computational Material Sciences
34	Mr. Prashil Badwaik	ICMS2026-C-60	<u>Molecular Simulation Studies of Enhanced Oil Recovery</u>	Computational Material Sciences
35	Dr. Manas Sharma	ICMS2026-D-2	<u>MLIP Studio: An Open Platform for Interactive Benchmarking and Atomistic Simulations Using Machine Learning Interatomic Potentials</u>	Machine Learning and AI, and Molecular Modeling

36	Mr. Rupendra Krishna Ganapathy Vydadi	ICMS2026-D-13	<u>Deep Learning and Molecular Modelling Enable the Rational Design of Nucleic Acid Aptamers Targeting Viral RNA Polymerases</u>	Machine Learning and AI, and Molecular Modeling
37	Mr. Mukul .	ICMS2026-D-14	<u>Effects of side chains of amino acids on CO2 capture: An Integrated Density Functional Theory-Machine Learning Approach</u>	Machine Learning and AI, and Molecular Modeling
38	Ms. Jahanvi Verma	ICMS2026-D-15	<u>MD simulations illuminate the destabilization mechanism of oligoquinoline-based foldamer against Aβ42 protofibrils</u>	Machine Learning and AI, and Molecular Modeling
39	Ms. Suruchi Bhambri	ICMS2026-D-16	<u>Targeting Cryptic Binding Sites in CDK12 Using Enhanced Sampling Molecular Dynamics and Artificial Intelligence-Driven Drug Discovery</u>	Machine Learning and AI, and Molecular Modeling
40	Mr. LIKUN PRADHAN	ICMS2026-D-17	<u>Development of Machine-Learning Interatomic Potential for Na⁺-ion Transport in NASICON Solid Electrolytes</u>	Machine Learning and AI, and Molecular Modeling
41	Ms. ISHA TANWAR	ICMS2026-D-19	<u>Insights into the myricetin-mediated inhibition of human calcitonin fibrillation using computer simulations</u>	Machine Learning and AI, and Molecular Modeling
42	Mr. Chiranjit Dutta	ICMS2026-D-21	<u>Computational Study of CrCl3 Nucleation in a PVTD Reactor</u>	Machine Learning and AI, and Molecular Modeling
43	Dr. Harini K	ICMS2026-D-28	<u>Computational analysis of the non-centromeric role of CenH3 chaperone in yeast</u>	Machine Learning and AI, and Molecular Modeling
44	Mr. Amal S	ICMS2026-D-4	<u>A Diffusion Model for Learning and Generating Realistic Metal–Organic Frameworks</u>	Machine Learning and AI, and Molecular Modeling
45	Mr. Devansh Sharma	ICMS2026-F-17	<u>State-to-State Transport Analysis: Unraveling Quantum Pathways in Molecular Aggregates</u>	Theory and Methodology
46	Mr. Daniel Zhang	ICMS2026-F-18	<u>Membrane Pore Formation Unveiled by 8RETIS Path Sampling: From Thinning to Flip-Flop</u>	Theory and Methodology
47	Mr. Appala Naidu Rayavarapu	ICMS2026-F-20	<u>Effect of Particle Size Distribution on Crystallization of Size-Disperse Hard Sphere Systems</u>	Theory and Methodology
48	Mr. Yeseong Choi	ICMS2026-F-21	<u>Multibath formulation of Thermalized Gaussian Wavepacket for Dynamics of Open Quantum Systems</u>	Theory and Methodology
49	Mr. Amal Krishna J	ICMS2026-F-23	<u>Ranking Anti-Agglomerant Performance in Gas Hydrate Systems Using Disjoining Pressure from Molecular Simulations</u>	Theory and Methodology
50	Mr. Shiva Sai Tadikonda	ICMS2026-F-24	<u>Quantitative assessment of dynamics-based kinetic parameter extraction using ChemXDyn</u>	Theory and Methodology
51	Dr. Tetsuro Nagai	ICMS2026-F-27	<u>Machine learning-aided coarse-grained dynamics simulations for gas diffusion in large-scale realistic systems</u>	Theory and Methodology
52	Dr. Manan Gupta	ICMS2026-F-19	<u>A Composite Kernel for Hilbert Space Projection of Gene Expression Data for Identification of Differentially Expressed Genes</u>	Theory and Methodology
53	Mr. Kazuki Yamauchi	ICMS2026-G-13	<u>Data-Driven Discovery of Entanglement Effects in Polymer Melts using Graph Neural Networks</u>	Polymers and Soft Matter
54	Mr. Ananta Sahoo	ICMS2026-G-15	<u>Stereo-Selective Supramolecular Polymerization of RR/SS-NDI: A Molecular Simulation Study</u>	Polymers and Soft Matter
55	Dr. Sheeba Malik	ICMS2026-G-18	<u>Molecular Insights into Lignocellulosic Biomass Delignification using Organosolv</u>	Polymers and Soft Matter
56	Ms. Mamta Yadav	ICMS2026-G-19	<u>Effect of protein binding and salt concentrations on the elastic properties of DNA: A Molecular Dynamics Study</u>	Polymers and Soft Matter
57	Mr. Venkatesh N	ICMS2026-G-20	<u>Structural Origin of Translational Jumps and Allied Dynamical Anomalies in Supercooled Water</u>	Polymers and Soft Matter
58	Ms. Kota Prathima	ICMS2026-H-2	<u>Evaluation of Additives for Enhanced CO₂ Capture Using Molecular Simulations</u>	Energy
59	Mr. Shubham Basera	ICMS2026-H-4	<u>Investigating Charge Transfer Pathways in the Photosystem I Reaction Center</u>	Energy
60	Mr. Shubham Chobe	ICMS2026-H-7	<u>How and Why Crude Oil Sticks to Rock Surface</u>	Energy
61	Dr. VISHNU SUDARSANAN	ICMS2026-H-9	<u>Effect of Lithium Intercalation Stages on the Adsorption of Electrolyte Solvents on Graphite Anodes: A DFT Study</u>	Energy
62	Dr. ABDULKAREEM U	ICMS2026-H-10	<u>Natural Gas Adsorption in Linker-Interconnected Graphene Oxide Porous Frameworks</u>	Energy
63	Mr. Nayan Dey	ICMS2026-H-11	<u>Effect of mixed EC/DMC solvent composition and temperature on structure and ion transport in a lithium bis(fluorosulfonyl)imide salt-based battery electrolyte</u>	Energy

DAY 3 - Wednesday, 07/10/2026

Poster Board No.	Name	Abstract ID	Title	Category
1	Mr. Shreyas Dindorkar	ICMS2026-A-67	<u>Development of an Additive CHARMM Force Field for Experimentally Informed Molecular Modeling of Bacterial Peptidoglycan</u>	Biological Systems and Medicine
2	Mr. Vikram R	ICMS2026-A-69	<u>A Molecular Simulation Study for Solvation Dynamics of Pharmaceutical Molecules</u>	Biological Systems and Medicine
3	Ms. Divya P	ICMS2026-A-72	<u>Thermodynamic and Kinetic Determinants of Antitubercular Activity in Imidazo[1,2-a] pyrimidine-Triazole Hybrids Revealed by Molecular Simulations</u>	Biological Systems and Medicine
4	Ms. SANGEETA KUMARI	ICMS2026-A-73	<u>Understanding the Inhibition of Arginase Active Sites by Carbon Quantum Dots through the Estimation of Structural Stability and Interaction Energies</u>	Biological Systems and Medicine
5	Mr. Aryan Lotake	ICMS2026-A-77	<u>Insights into Antimicrobial Peptide Disruption Mechanisms on Bacterial Membranes</u>	Biological Systems and Medicine
6	Mr. Bilash Maity	ICMS2026-A-79	<u>Uncovering the Molecular Basis of Glycosylated Peptide Aggregation</u>	Biological Systems and Medicine
7	Mr. Shrivnandi	ICMS2026-A-82	<u>Amyloid Oligomers under Crowding: Role of Crowder Size and Chemistry</u>	Biological Systems and Medicine
8	Ms. Arpita Khamle	ICMS2026-A-83	<u>Rational Design of a CagA Mimicking Peptide as a Broad-Spectrum Amyloid Aggregation Inhibitor</u>	Biological Systems and Medicine
9	Ms. Varshini Kore	ICMS2026-A-84	<u>A Mutation-Induced Cryptic Allosteric Pocket Drives Ceftazidime-Avibactam Resistance in D179Y KPC-2: Insights from Microsecond Molecular Dynamics Simulations</u>	Biological Systems and Medicine
10	Mr. ABHISHEK LAKHERA	ICMS2026-A-85	<u>Molecular Dynamics Simulations Reveal Evolutionary Remodeling of SARS-CoV-2 Spike Interactions with ACE2, Fibrinogen, and Neutralizing Antibodies</u>	Biological Systems and Medicine
11	Mr. Roman Tsiniavskii	ICMS2026-A-90	<u>Molecular dynamics study of temperature induced transition in haemoglobin and its hydration shell</u>	Biological Systems and Medicine
12	Mr. Ravishankar Srivastava	ICMS2026-A-91	<u>Integrative Simulation and Spectroscopy Illuminates L-asparaginase Stability on Nanocomposite Surfaces for Biosensing</u>	Biological Systems and Medicine
13	Mr. Reshob Routh	ICMS2026-A-97	<u>Cryptic Residue-Guided Mutation Enables Recovery of Ligand-Compatible Holo-Like Conformations</u>	Biological Systems and Medicine
14	Mrs. Muskan Agrawal	ICMS2026-A-119	<u>Designing Chameleonic β-Hairpin Antimicrobial Peptides for Selective Targeting of Bacterial Membranes</u>	Biological Systems and Medicine
15	Mr. Roni Saiba	ICMS2026-A-120	<u>STRUCTURAL AND MECHANICAL CHANGES IN BACTERIAL MEMBRANES CAUSED BY ANTIMICROBIAL AGENTS</u>	Biological Systems and Medicine
16	Pranjal Sur	ICMS2026-A-121	<u>Localized Electric-Field Signatures Enhance Peptide Discrimination in Nanopore Translocation</u>	Biological Systems and Medicine
17	Dr. Aziza Rahman	ICMS2026-A-243	<u>1:3 enzyme-substrate stoichiometry for cytochrome P450 (CYP3A4) binding to caffeine substrates</u>	Biological Systems and Medicine
18	Mr. Adarsh Tiwari	ICMS2026-A-123	<u>Analyzing the role of natural products in promoting or inhibiting NDP52 protein using molecular docking and dynamic simulation studies</u>	Biological Systems and Medicine
19	Mr. Amal Krishna J	ICMS2026-C-44	<u>Computational Screening of Combined I_2/CH_4 Capture in Nanoporous Materials under Humid Mixed-Gas Conditions</u>	Computational Material Sciences
20	Ms. AISHWARYA K	ICMS2026-C-61	<u>Developing Machine learning Interatomic potential for Iron phosphate glass</u>	Computational Material Sciences
21	Mr. Pritam Chakraborty	ICMS2026-C-62	<u>Towards the Formation of Porous Architecture via Self-Assembly of Anti-aromatic Dibenzopentalene - A Computational Study</u>	Computational Material Sciences
22	Ms. Jannat Alam	ICMS2026-C-63	<u>Plausible Stabilization of Anti-Bredt Olefins via Confined Chemistry - A Computational Study</u>	Computational Material Sciences
23	Ms. Neenu Joseph	ICMS2026-C-65	<u>Selectivity and Switchability of Hot Spot Activation in Nanolens-like Nanosphere Heterotrimers</u>	Computational Material Sciences
24	Ms. Aswathy R	ICMS2026-C-66	<u>Twist Induced Chiroptical Response in Stacked Triangular Nanoprism Dimers: Leveraging the Lightning-rod Effect</u>	Computational Material Sciences
25	Mr. Sourmyadeep Mukherjee	ICMS2026-C-68	<u>Modelling polaron binding energy in lithium peroxide (Li2O2) using long-range corrected methods</u>	Computational Material Sciences
26	Ms. Arzoo Rai	ICMS2026-C-69	<u>Selective Recognition of Alkali Metal Ions by Azocalix[4]arene-Based Quinone Receptors: A DFT Study</u>	Computational Material Sciences
27	Mr. Akshay Sriraman	ICMS2026-C-70	<u>Physics-Informed Sampling for MLIPs</u>	Computational Material Sciences
28	Dr. Deepak Gorai	ICMS2026-C-71	<u>Nitrogen Reduction Pathways on Transition Metal Electrocatalysts: A DFT Analysis</u>	Computational Material Sciences

29	Ms. Diksha Kadre	ICMS2026-C-76	<u>Computation of Free-Energy Landscape of Methane Hydrate Nucleation using Hybrid Monte Carlo Simulations</u>	Computational Material Sciences
30	Mr. Chaitanya Shah	ICMS2026-C-83	<u>Calculation of Free Energy Landscape for Nucleation of Amorphous Calcium Carbonate</u>	Computational Material Sciences
31	Mr. SIMPAL KUMAR SUMAN	ICMS2026-C-85	<u>BandGap-IN: An Integrated Computational Platform for Bandgap Calculation, Defect Analysis, and Property Modelling of Nanomaterials</u>	Computational Material Sciences
32	Mr. Klinton K	ICMS2026-C-86	<u>Orbital Hybridization and Electronic Correlation Effects in NbMnZ (Z = Ge, Sn) ferromagnetic Heusler Alloys for Spintronic and Thermoelectric Applications</u>	Computational Material Sciences
33	Dr. Sachin Gautham MB	ICMS2026-C-87	<u>Sorbent Design via Molecular Simulation for Atmospheric Water Harvesting</u>	Computational Material Sciences
34	Dr. Abhijit Gogoi	ICMS2026-C-98	<u>Atomistic Modeling of Nano-Organic Light-Emitting Diodes.</u>	Computational Material Sciences
35	Ms. Jampala Pasyanthi	ICMS2026-C-99	<u>Development of fully ab initio classical force fields for graphene: Applications to mechanical and interfacial properties</u>	Computational Material Sciences
36	Mr. Sanuja Khuntia	ICMS2026-C-77	<u>What drives structural distortions in two-dimensional hybrid halide perovskites?</u>	Computational Material Sciences
37	Mr. Guruswaroop C	ICMS2026-D-30	<u>Topological Modeling of KRAS Landscapes: How G12D Mutation Traps Switch Dynamics</u>	Machine Learning and AI, and Molecular Modeling
38	Ms. Haritha P	ICMS2026-D-31	<u>Probing the Molecular Mechanism of AIB-Mediated β-Sheet Disruption in Phenylalanine-Rich Heptapeptides Using Machine Learning Collective Variables</u>	Machine Learning and AI, and Molecular Modeling
39	Mr. Junsoo Lee	ICMS2026-D-33	<u>Charge-aware machine-learning molecular dynamics with dynamic Born effective charges for field-driven ferroelectric switching</u>	Machine Learning and AI, and Molecular Modeling
40	Ms. Pavani Tella	ICMS2026-D-41	<u>Mechanic insights of site-specific phosphorylation mediated modulation in p16/CDK4 binding dynamics using molecular simulation</u>	Machine Learning and AI, and Molecular Modeling
41	Dr. Ayushi Chauhan	ICMS2026-D-48	<u>Digital twin skin model to measure energy barrier and visualize the penetration of active through skin layer</u>	Machine Learning and AI, and Molecular Modeling
42	Dr. Kousika A	ICMS2026-D-77	<u>Investigating the Interfacial Properties of Defective hBN-Water Systems Using Neutral Network Potentials.</u>	Machine Learning and AI, and Molecular Modeling
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44	Dr. Hridya Valia Madapally	ICMS2026-D-200	<u>Integrating Generative AI and Physics-Based Refinement for High-Fidelity Ligand Pose Prediction in Flexible Receptor Environments</u>	Machine Learning and AI, and Molecular Modeling
45	Ms. Joshri G	ICMS2026-D-42	<u>A DFT-Informed, NLP-Curated Pipeline for Predicting Enantioselective Binding of Chiral Drugs in Cyclodextrin Systems</u>	Machine Learning and AI, and Molecular Modeling
46	Ms. Abhilasha Kumari	ICMS2026-F-28	<u>A new method to compute three-particle configurational entropy of simple fluids</u>	Theory and Methodology
47	Dr. Hyun Tae Jung	ICMS2026-F-30	<u>Direct Coupling of Fluctuating Hydrodynamics and Kinetic Monte Carlo for Gas-solid Interfacial Systems</u>	Theory and Methodology
48	Dr. Yuki Mitsuta	ICMS2026-F-31	<u>Automated Search Method of Free Energy Reaction Networks on Multi-dimensional Free Energy Landscapes</u>	Theory and Methodology
49	Mr. Ikki Takahashi	ICMS2026-F-32	<u>Extended Hertzian Framework for Contact Area Estimation of Polymer Particle beyond the Elastic Limit</u>	Theory and Methodology
50	Mr. Shuto Saeki	ICMS2026-F-33	<u>A methodology of efficiently computing solvation free energy with a solute electronic state</u>	Theory and Methodology
51	Mr. Nishant Gupta	ICMS2026-F-37	<u>First-Principles Modeling of Electrochemical Systems using Finite-Element DFT Calculations</u>	Theory and Methodology
52	Mr. Ryo Okabe	ICMS2026-G-29	<u>Analysis on ion-transport in a crosslinked polymer membrane using all-atom MD simulation</u>	Polymers and Soft Matter
53	Mr. Prabeen Pattnayak	ICMS2026-G-30	<u>When intramolecular topology affects macromolecular diffusion in dilute solutions</u>	Polymers and Soft Matter
54	Mr. Kohei Yoshikawa	ICMS2026-G-31	<u>Identifying Structural Descriptors of Liquid Water Across Temperatures Using Machine Learning</u>	Polymers and Soft Matter
55	Mr. Keishin Tsujino	ICMS2026-G-32	<u>Elucidating the Breakdown of Cox-Merz Rule in Linear and Ring Polymer Melts</u>	Polymers and Soft Matter
56	Mr. MOHD BASEER	ICMS2026-G-23	<u>WATER RETENTION AND CLUSTER DYNAMICS IN LIPID BILAYER HYDROPHOBIC CORES: A MOLECULAR DYNAMICS STUDY</u>	Polymers and Soft Matter
57	Dr. Monmee Phukan	ICMS2026-G-56	<u>Density-driven reentrant polymer transitions via saturable bridging crowders</u>	Polymers and Soft Matter

58	Dr. Dibyendu Bandyopadhyay	ICMS2026-G-21	<u>Correlation Between Pair Excess Entropy, Hydrogen-Bond Network, and Molecular Mobility in Common Water Models: A Molecular Dynamics Study</u>	Polymers and Soft Matter
59	Ms. Itipragnya Pati	ICMS2026-H-13	<u>Solvation Shells as Descriptors for Ion Transport in Sodium-Ion Battery Electrolytes</u>	Energy
60	Mr. Abhigyan Hazarika	ICMS2026-H-14	<u>Memory effects influence ice growth in the non-equilibrium freezing of water</u>	Energy
61	Mrs. Kalyani Mohanty	ICMS2026-H-16	<u>Interfacial Structure and Charge Storage Mechanisms of Ti3C2Tx MXene in BMIM-PF6 Ionic Liquid</u>	Energy
62	Ms. Soumyashree Adhikari	ICMS2026-H-17	<u>Understanding Na+ Solvation Chemistry in NaFSI-Based PC/EC Electrolytes from Dilute to Localized High-Concentration Conditions</u>	Energy
63	Mr. Riku Kitano	ICMS2026-H-18	<u>Reinterpretation of the Stokes–Einstein relation in Li+ electrolytes using molecular dynamics simulations</u>	Energy
64	Ms. Anushka Venkatesh	ICMS2026-H-20	<u>Chemical Reactivity under Thermochemical Non-Equilibrium: A Reactive Molecular Dynamics Study</u>	Energy