List of Posters

Sr. No.	Code	Presenting Author	Title
P1	A-1	Sabarish T S	Physics-Informed Neural Network Assisted X-ray and Photoacoustic Characterization of Thermally Aged Zircaloy-2 for Predictive Thermal Property Evaluation
P2	A-4	Kamal Nayan Goswami	Influence of lithium vacancy defects on tritium diffusion in β-Li_2TiO_3: a first-principles study for fusion breeder blankets
P3	B-1	Vemuri Lakshmi Ganesh	The Effect of Cyclic groups in Uranium Extraction: A Computational Study
P4	B-3	Haseen Siddiqui	Temperature-dependent mechanistic insights into CO_2 hydrogenation to methanol on Cu (111): A DFT-assisted micro-kinetic study
P5	B-4	Srijita Chakraborty	DFT-Based Modeling of Lanthanide Double PerovskitesR_2NiIrO_6 (R = Pr, Nd): Electronic Structure and Effects of Lattice Distortion and Spin-Orbit Coupling
P6	C-2	Satyam Shree	Length-Dependent Anomalous Water Transport in Carbon Nanotube Membranes: A Molecular Dynamics Study
P7	C-4	Akula Deepchander	Understand the Molecular-level insight into the interfacial and phase equilibrium properties of CO_2 + R1234yf refrigerant blend
P8	C-5	A K Singha Deb	Glucose-functionalized MOFs for Boron Separation from aqueous solution: Synthesis, Adsorption and DFT study
P9	C-6	Sayantan Maity	Modelling of Li-ion capture over Na-ion by a LMWG
P10	C-7	I. Mohanakkaviya	Exploring the Relationship between Network Architecture and Water Transport in Polyimine Membranes: A Molecular Dynamics Study
P11	C-8	Vikram Ramalingam	Unraveling CO_2 Hydrate Formation: The Molecular Role of Additive Concentration
P12	C-9	Raghibul Hussain	Density Functional Theory based Investigation about Adsorption and Dissociation of Oxygen on Copper Surface of Different
P13	C-10	Fathima Thasleem M S	Effect of Dispersion On The Adsorption of Xenon, Krypton And Water With Different Metal Organic Frameworks
P14	C-11	Binu Varghese	Selective Rejection of Uranyl Ions from Sea Water Using Covalent Organic Framework Membranes
P15	D-1	K. B. Nerkar	Tuning Hydrogen Storage in Metal-Decorated Nanocages through Heteroatom Concentration: A DFT Study
P16	D-2	Saumyajeet Mukherjee	DFT Study on the Adsorption of Hydrogen and Deuterium on Platinum-111 Surface
P17	D-3	S. Elavarasan	Structural and Morphological Properties of Hydrothermally Synthesized Pure and Sm-Doped SnO_2 Nanoparticles
P18	D-4	Aritri Roy	Atomistic Modelling of Local-Field Effects in Catalysis
P19	D-5	Suvarna Vincent	Tuning Hydrogen Adsorption and Storage in C5N Monolayers through Light-Metal Decoration: A First-Principles Study
P20	D-6	M L Murchana Kalita	Computational Screening of Transition Metal Containing 2D MOF for CO2 Reduction Reaction
P21	D-8	Saikat Saha	Connecting Reaction Pathways, Kinetics, and Selectivity in Furfural Conversion over Transition Metals: A DFT–MKM Approach
P22	D-12	Sosanna Mathewa	Investigating Ion Transport Behavior in Nafion Under Electric Fields for Improved Hydrogen Production in Cu–ClElectrolyzer
P23	E-2	Joyael Anthikkatt	First-Principles Investigation of Novel 2D C_2O Crown Ether as Anode Material for Lithium-Ion Batteries

P24	E-5	Anupama Shaju	$MgTiO_3$ Nanoparticles as a Functional Electrode Material for Electrochemical Energy Storage
P25	E-6	Reman Rana	Structural, Electronic, Thermal and Dynamical studies on zeta-V_2O_5 as a potential cathode material: Insights from Density Functional Theory
P26	G-1	Abinaya.V.	First-Principles and Molecular Dynamics Study of Functionalized Aluminum Nitride Nanotubes for Capecitabine Delivery
P27	G-3	Sumit Sharma	Molecular Dynamics Simulation of Polyurea Adhesion on Metal Oxides: Substrate Chemistry, Crystallography, and Surface Cation Interaction
P28	G-4	Sneha. J	Computational Insights into the Covalent Functionalization of Boron Nitride Nanotube with Essential Amino Acids for Thymoquinone Delivery
P29	G-5	Mansi Jain	Deciphering Ionic Conductivity Differences in Linear Carbonate Electrolytes: Conformational Shrinkage and Solvation Structure in Dimethyl vs Diethyl Carbonate
P30	G-6	Rakhi Katyal	Diffusion power laws in hydrated biopolymer electrolytes
P31	G-8	Sonam Bansal	Teaching Research-Based Modelling: A Pedagogical Framework for PhD Education in Molecular Chemistry
P32	G-10	Manisha Kumari Meena	Hydration Effects on Ion Solvation Shell Structure in ssDNA-Ionic Liquid Electrolytes
P33	G-11	Sheetal Sisodiya	First-Principles Investigation of Vibrational and Optical Properties of Pristine and Pd-Decorated C120 Carbon Nanotubes
P34	G-12	Venkatesh Nagaraj	Structural Origin of Translational Jumps and Allied Dynamical Anomalies in Supercooled Water
P35	H-1	Harini Saravanan	Understanding Electrostatics at Charged Metal-Water Interface using 2D Coulomb Kernel Truncation and Machine Learning Force Fields
P36	H-2	Suman Mondal	Machine-Learned Potentials for Radiation Damage in Tantalum
P37	H-3	Akshay Sriraman	Reactive Hydronium–Hydroxide Sampling and Proton-TransferBarrier Benchmarks for Machine-Learned Grotthuss Kinetics
P38	H-5	Nancy Semwal	Fine-tuning universal machine-learning interatomic potentials for adsorption isotherms: UMA-S on Mg-MOF-74
P39	H-10	Pritam Rudra	Predicting Thermophysical Properties of Halide Salts Using On-the-Fly Machine-Learned Interatomic Potentials across Multiple Exchange-Correlation Functionals
P40	H-11	Satabdi Roy	Physics-Informed Machine Learning-Based Generative Configurational Sampling of Glass-Forming Liquids
P41	H-13	Molly Mehra	Performance Benchmarking and Qubit Scaling of Variational Quantum Eigensolver Simulations on Multicore CPU System
P42	H-15	Hafijullah Khan	Robust Machine Learning Interatomic Potentials for Heterogeneous Environment in Catalysis
P43	H-16	Anjana Tripathi	Coverage-Driven Machine Learning Framework for the Rational Design of High-Entropy Alloy Electrocatalysts
P44	H-17	Bharathi S	A Single-Valued NeutrosophicAczel–Alsina Power Prioritized Aggregation-Based MADM Approach for Renewable Energy Company Selection
P45	H-18	Janvi Semwal	AViML: Machine Learning-Based Defect and Microstructure Characterization in Atomistic Simulations
P46	I-3	S.G. Khambholja	Electrical transport properties of liquid K-Pb alloys
P47	J-1	Snehasish Barman Roy	Model-based pulse amplitude determination in two-phase flow condition in pulsed sieve plate column

P48	J-2	Ankit Badiwal	ANUSim module to simulate the decomposition of ammonium nitrate in a fluidized bed reactor
P49	J-5	Hisham Kurikkal M. T.	2D axisymmetric CFD model of an air-pulsed dissolution vessel
P50	J-6	Saurav Bhattacharya	CFD multiscale simulation study of HI decomposer in Iodine sulfur process
P51	K-2	A. Potti	Modelling of a Novel Integrated Jacketed Spray Dryer System with MVR for Efficient $CuCl_2$ Drying in the Cu-Cl Cycle
P52	L-1	Ankit Ojha	Modelling of bulk thermal polymerization of styrene
P53	M-1	Kshitij Asit Acharya	Assessment of OFFBEAT for PHWR fuel: Investigative benchmark study on the IAEA FUMEX-II CANDU cases
P54	N-1	Projesh Kumar Roy	Computational study of the fibrillation inhibition mechanism of Hen Egg White Lysozyme protein using Pluronics
P55	N-2	Sanskruti Ramprasad Mishra	Can Substituents Control the Interaction Pattern? A Switch between Osme and Hydrogen Bond
P56	N-3	Sandeep Singh Tomar	Mathematical Modeling of Concentration Overpotential in CuCl/HClElectrolyzer for Hydrogen Production in Copper-Chlorine Thermochemical Cycle
P57	N-5	Preeti Tripathi	Biophysical Characterization of Plasmodium falciparum Ribosomal Protein P2: Oligomeric Behaviour, Structural Stability and Nucleic-Acid-induced Fluorescence Changes
P58	N-6	Dhruvakumar T K	Prediction of Sauter mean droplet diameter using Light Gradient Boosting Technique
P59	N-8	Simpal Kumar Suman	BandGap-IN: An Integrated Software for Nanomaterial Bandgap Modeling, Defect Analysis and Visualization
P60	N-9	A Abhijith	Defect Evolution in Equiatomic and Non-EquiatomicNbTaVTi Multi-Principal Element Alloys under Uniaxial Tension and Compression: A molecular dynamics study
P61	N-10	Chintak Kamalesh Parashar	Recipes for mixing vortices in a microchannel using electric field
P62	N-11	Anagha Das	Inducing Magnetism in Newly Synthesised $NbOCl_2$ via Non-Metal (B, C, N) Doping: A First-Principles Study
P63	N-12	Ananta Krushna Sahoo	Stereo-Selective Supramolecular Polymerization of RR/SS-NDI: A Molecular Simulation Study
P64	N-13	Soumyadip Mondal	Modelled isotherm based RDC generated data correlated with drop size distribution model
P-65	N-22	Anwesha Chakraborty	Spin fluctuation mediated superconductivity in doped iron-based superconducting systems