

## List of poster presenter in ICMG – III (2024)

Reg. No	Poster Number	Full Nama	Affiliation	Title
ICMG-III-P01	P01	Aathira Nair	CSIR National chemical laboratory, Pune	What leads to direct epoxidation? An exhaustive DFT investigation of electrophilic oxygen mediated epoxidation of ethylene on Ag(100)
ICMG-III-P02	P02	Amaze Mathe	Vignan's Foundation for Science, Technology & Research, Guntur	Computational Investigation of the Binding Affinity of 7,9-Di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione with Cyclooxygenase Enzymes: A QM/MM Study
ICMG-III-P03	P03	Anamika Roy	Charuchandra College, Kolkata; St. Xavier's College, Kolkata	Studying dynamics of collective motion from topological perspective
ICMG-III-P04	P04	Anju Rajan	NIT Calicut	First-principle investigation of Janus SnSSe as a promising material for NO, NO <sub>2</sub> and NH <sub>3</sub> gas sensing.
ICMG-III-P05	P05	Archan Ravi Sankar	PhD, VIT University, Chennai	A Computational Study to Determine the Role of $\sigma$ -Hole in nido-Heteroborane Binding Capabilities
ICMG-III-P06	P06	Ashok Singh	Indian Institute of Technology Indore	Synergistic Niobium Doped Two-Dimensional Zirconium Diselenide: An Efficient Electrocatalyst for O <sub>2</sub> Reduction Reaction
ICMG-III-P07	P07	Asif Iqbal	SRM University AP, Andhra Pradesh	C <sub>2</sub> product formation over C <sub>1</sub> product and HER on 111 plane of specific Cu alloy nanoparticle identified through

				multiparameter optimization
ICMG-III-P08	P08	Atish Kumar Sharma	P.G. Department of Physics, Samastipur College, Samastipur-848134 (A constituent unit of L.N.M.U. Darbhanga-846004), Bihar, India.)	Comprehensive impedance and admittance spectroscopic investigation of MoS <sub>2</sub> -solar cells with exclusive Zn <sub>3</sub> P <sub>2</sub> as HTL and least lattice mismatches
ICMG-III-P09	P09	Ayusmin Panda	IIT Madras	Enhancement of Quantum Efficiency in Perovskite Solar Cells through Whispering Gallery Modes from Titanium Oxide Micro-resonators
ICMG-III-P10	P10	Babuji Dandigunta	Indian Institute of Technology, Madras	$\alpha$ -Graphyne with Ultra-low Diffusion Barriers as a Promising Sodium-ion Battery Anode: Ab-initio DFT and MD Studies
ICMG-III-P11	P11	Deeksha R	M.S. Ramaiah University of Applied Sciences	Unveiling the Synergistic Performance of Double-atom Transition Metal Incorporation in Graphitic Surfaces as Electrocatalysts
ICMG-III-P12	P12	Dr Thulasi Bikku	Amrita Vishwa Vidyapeetham	Improved Quantum Algorithm: A Crucial Stepping Stone in Quantum-Powered Drug Discovery
ICMG-III-P13	P13	Dr. Charan Kuchi	Madanapalle Institute of Technology and Science, Madanapalle, 517325, India.	Synergistic MoS <sub>2</sub> -TiO <sub>2</sub> Nanocomposite for Efficient H <sub>2</sub> Evolution, Dye Degradation, and Supercapacitor Applications
ICMG-III-P14	P14	Dr. Jagadish Chandra Mahato	Siksha Bhavana, Visva Bharati, Santiniketan-731235, West Bengal, India	Unveiling the potential of two-dimensional V <sub>2</sub> S <sub>2</sub> monolayer as a high-performance anode material for metal-ion batteries: A first-principles study

ICMG-III-P15	P15	Golam Rosul Khan	IIT Patna	What is the viscosity of liquid water confined in a hydrophobic nanotube? Estimation using a novel approach
ICMG-III-P16	P16	Himani Joshi	Indian Institute Of Technology, Indore	Unveiling the Electrocatalytic Activity of Cobaloxime Metallolinker in UU-100(Co) Metal-Organic Framework towards H <sub>2</sub> Evolution Reaction: A DFT Study
ICMG-III-P17	P17	Ishita Ghorai	IIT Mandi	Quantum monodromy in effective polyad breaking Hamiltonian
ICMG-III-P18	P18	Jesni M Jacob	SRM -AP	Theoretical Insights into Impact of Solid-State Environment on hot-exciton TADF Emitter Properties
ICMG-III-P19	P19	Jishnu Sai Gopinath	National Institute of Technology Calicut	CARBONE SUPPORTED DIBERYLLIUM COMPOUNDS Be <sub>2</sub> (CL <sub>2</sub> ) <sub>2</sub> , L=NHC, PMe <sub>3</sub> , cAAC and CO A THEORETICAL STUDY
ICMG-III-P20	P20	Jose Antony V J	CUSAT	Tri-Atom Metal Cluster Decorated Nb <sub>2</sub> CO <sub>2</sub> MXene: Comparative Insights for Efficient Hydrogen Evolution Reaction
ICMG-III-P21	P21	K M Rajashekhar Vaibhava	Poornaprajna Institute Of Scientific Research	Treatment of Van der Waals dispersion forces for layered MXenes in the framework of DFT
ICMG-III-P22	P22	K. Santhy	Indus University, Ahmedabad	Experimental Investigation and Thermodynamic Reassessment of Mg-Sr-Zn Ternary System
ICMG-III-P23	P23	Karthik H J	PhD Scholar	Semiconductor to Metal transition in single and double polyyn chains

ICMG-III-P24	P24	Kushal Samanta	Indian Institute of Technology, Delhi	Atomistic Insights on FacetDependent Functional Properties in CdSe Nanocrystals
ICMG-III-P25	P25	Likun Pradhan	IIT Guwahati	Atomistic simulation studies of ion transport in NASICON using molecular dynamics simulations
ICMG-III-P26	P26	M Bhargavi	SRM University AP, Andhra Pradesh	Enriched Optical Dielectric and Magnetic Properties of Praseodymium and Bismuth substituted Yttrium iron Garnet (Pr: BYIG) nanoparticles by sol-gel Technique
ICMG-III-P27	P27	Madhavan Nampoothiri D K	Indian Institute of Science, Bangalore	Understanding the effect of O <sub>2</sub> in the growth mechanism of 2D MoS <sub>2</sub> in a chemical vapor deposition reactor
ICMG-III-P28	P28	Mahima Bhardwaj	Vignan's Foundation for Science, Technology and Research, Vadlamudi, Guntur-522213, Andhra Pradesh, India	Prediction of significant biomarkers by network analysis for breast cancer bone metastasis
ICMG-III-P29	P29	Maneesha M	Cochin University of Science and Technology	An Understanding into the CO <sub>2</sub> Reduction on Homo and Hetero atom doped V <sub>2</sub> CO <sub>2</sub>
ICMG-III-P30	P30	Meema Bhati	CSIR-NCL, Pune	Traversing the role of nonpolar surfaces of ZnO in industrial catalysts form CO <sub>2</sub> reduction to methanol synthesis: A Periodic DFT Investigation
ICMG-III-P31	P31	Muhammed Fasil P P	NIT Calicut	Enhanced Catalytic Activity in Nb-Doped TiO <sub>2</sub> for Electrochemical Oxygen Reduction Reaction

ICMG-III-P32	P32	Narad Barman	SRM University AP, Amaravati, Andhra Pradesh	Charge contortion due to bridge oxygen vacancy in SnO <sub>2</sub> lattice manipulate the nature of N <sub>2</sub> adsorption towards a kinetically-driven ammonia electrosynthesis
ICMG-III-P33	P33	Nidhi	Delhi Technological University, New Delhi 110042	A first-principles study of the topological phase in Zintl compound KCd <sub>4</sub> As <sub>3</sub>
ICMG-III-P34	P34	Nikhil Wilson	CSIR-NCL	HYST 2.0: Analysis and interpretations of machine learning model trained on an updated database
ICMG-III-P35	P35	Nilofar Naaz	BITS Pilani Hyderabad Campus	Effect of Mn Doping on the Electrical Conduction Properties of BiFeO <sub>3</sub> Thin-Films
ICMG-III-P36	P36	Pallavi Vyankuram Chame	Department of Chemistry, Indian Institute of Science Education and Research Pune	Water dissociation on (0001) surface of $\alpha$ -Titanium: a first principles investigation.
ICMG-III-P37	P37	Pramod Kumar Verma	Indian Institute of Technology Madras	A Real-Time Study of Charge-Transfer Dynamics in Metal Nanoparticle-Perfluorooctaniod Acid (PFOA) and Degradation of PFOA
ICMG-III-P38	P38	Rajeev Ranjan	IISER Pune	Entropy stabilized HfZrNiCoSnSb half-Heusler alloy for thermoelectric application: a theoretical prediction
ICMG-III-P39	P39	Rakesh Kumar	Lalit Narayan Mithila University, Darbhanga -Bihar	First principle studies of novel Mg(NH <sub>2</sub> ) <sub>2</sub> and LiH for enhancing kinetics for hydrogen storage along with LiBH <sub>4</sub> as additive under the ambient condition
ICMG-III-P40	P40	Ramesh Kumar	Delhi Technological University	An ab-initio study of topological phase tuning in Zintl compound RbZn <sub>4</sub> P <sub>3</sub>

ICMG-III-P41	P41	Sai Raj Ali	Jamia Millia Islamia University, New Delhi	Unlocking the Potential of $\text{Mo}_2\text{CO}_2$ MXenes for the Hydrogen Evolution Reaction via Single Atom Doping.
ICMG-III-P42	P42	Sairathna Choppella	SRM University AP, Andhra Pradesh	Non fullerene acceptors with Enhanced Photostability for Organic Solar Cells applications
ICMG-III-P43	P43	Samir Kumar Nayak	IIT Madras	Computing accurate bond dissociation energies of emerging per- and polyfluoroalkyl substances: Achieving chemical accuracy using connectivity-based hierarchy schemes
ICMG-III-P44	P44	Sangeeta	Delhi Technological University, Delhi	Exploring the Thermoelectric Potential of $\text{CsGaSb}_2$ Zintl Phase Compound: A Computational Study
ICMG-III-P45	P45	Sanjib Ray	IIT Guwahati	Role of framework flexibility and local cationic environments on oxide ion transport in Sr-doped $\text{LaFeO}_3$
ICMG-III-P46	P46	Sourav Ghosh	SRM University AP, Andhra Pradesh	Bond Exchange Mechanism Drives Volmer-Tafel route and Electronic Descriptor to Predict HER Activity of Borophene
ICMG-III-P47	P47	Stephen .S Mathew	Delhi Technological University	The Impact of Strain on the Thermoelectric Properties of $\text{HfNBr}$ Monolayer: A First-Principles Study
ICMG-III-P48	P48	Sudipta Roy	Department of Physics, IISER Pune	Efficient Water–Gas shift catalysts for $\text{H}_2\text{O}$ and $\text{CO}$ dissociation using $\text{Cu–Ni}$ step alloy surfaces
ICMG-III-P49	P49	Sushri Soumya Jena	Birla Institute of Technology and Science, Pilani	Understanding Ammonia Gas Sensing Mechanism

				in n-Type Conducting Polymer
ICMG-III-P50	P50	Tangudupalli Mahesh Kumar	SRM University AP, Andhra Pradesh	Applicability of Polyurethane Foam Filled Thin-Walled Composite Columns in Structural Engineering
ICMG-III-P51	P51	Thillaiarasi S	SRM University AP, Andhra Pradesh	Enhancing Photochemical Reactivity and Large Solar Thermal Energy Storage with Polycyclic Heteroaromatic $\pi$ -Linkers in Dithienylethene Molecular Switches
ICMG-III-P52	P52	Uday Kumar M	Department of Physics, B.M.S College of Engineering, Bengaluru	Substantial enhancement of thermoelectric power factor of undoped CoSb <sub>3</sub> Skutterudites processed by microwave sintering
ICMG-III-P53	P53	Vivek Pandey	SRM University AP, Andhra Pradesh	Longitudinal Interband Conductivity in Dirac Nodal Line Semimetals: Intrinsic and Extrinsic contributions
ICMG-III-P54	P54	Bodaballa Narendra Kumar	SRM University AP, Andhra Pradesh	Temporal Evolution of Avalanches in the Fiber Bundle Model of Disordered Solids
ICMG-III-P55	P55	Diksha	SRM University AP, Andhra Pradesh	Prediction of imminent breakdown using Gini and Kolkata indices
ICMG-III-P56	P56	Gunnemeda Eswar	Bsc physics (Hons) SRM University AP, Andhra Pradesh	Understanding the dynamics of driven interfaces through disordered media is crucial for various systems,
ICMG-III-P57	P57	Kandalam Ravitheja	SRM University AP, Andhra Pradesh	Understanding the effect of alignment interaction on spatio-temporal patterns in a active matter system.
ICMG-III-P58	P58	Ruhul Amin Ibne Haque	St. Xavier's College	Fracture Networks: Topology, Geometry and Evolution
ICMG-III-P59	P59	Soumyaditya Das	SRM University AP, Andhra Pradesh	Critical properties and scaling through Gini index

ICMG-III-P60	P60	Subhajit Gupta	SRM University AP, Andhra Pradesh	Viscoelastic effect on oscillation and synchronization of biological oscillators
ICMG-III-P61	P61	Tarun Ram Kanuri	SRM University AP, Andhra Pradesh	Studying the final values of inequality indexes for creep ruptures using the fiber bundle model
ICMG-III-P62	P62	Viswakannan R K	Birla Institute of Technology and Sciences Pilani, Hyderabad Campus	Critical crack length during fracture