AAPALI PSI-K 2025

May 19 - 21, 2025, IISER Pune, India

Schedule of poster presentation

DAY 1: May 19, 2025			
Poster No:	**Name**	**Affiliation**	**Title**
1	Ankita Kumari	Indian Institute of Technology Delhi, Department-Chemistry	Ultrafast Dynamics of Photogenerated Electrons at NO3/CdSe QD Interface Driven by Capture of Hot Electrons-Ab Initio Quantum Dynamics Simulation
2	Akanksha Sharma	Chemistry Department, Indian Institute of Technology, Delhi, New Delhi	Pressure-Induced Modulation of Structural and Optoelectronic Properties in 2D Halide Perovskites: Insights from Ab Initio Molecular Dynamics Simulations
3	Ankita	Department of Chemistry, IIT Madras	Interfacial stability of Electrolytes at pure and oxidized Mg surfaces- Insights from Ab Initio Molecular Dynamics
4	Anwesha Chakraborty	Homi Bhabha National Institute, Anusaktinagar, Mumbai-400094, India	Effect of anionic and cationic doping on Fe-based superconducting series: interplay of magnetism and superconductivity
5	Anwesha Das	Jawaharlal Nehru Centre For Advanced Scientific Research, Theoretical Sciences Unit	First Principles Analysis of In-Plane Heterostructure of 2D Materials
6	ATHIRA K K	DEPARTMENT OF CHEMICAL ENGINEERING, IIT MADRAS, CHENNAI, TAMILNADU, 600036	Computational and Experimental Investigation of Morphology and Metal Ions Influence of ZIFs in CO_2 Cycloaddition Reactions
7	Bhawna	Chemistry Department (IIT Delhi)	Tuning Hot Carrier Dynamics in Vacancy-Ordered Halide Perovskites through Lattice Compression: Insight from ab initio Quantum Dynamics and Machine Learning
8	Dimple Rani	School of Physical Sciences, NISER Bhubaneswar	Thermoelectric characteristics of silver-based semiconductors using the non-empirical range-separated dielectric-dependent hybrid
9	DOLAN ACHARYA	Department of Physics, National Institute of Technology Durgapur, Mahatma Gandhi Avenue, Durgapur, West Bengal, India, PIN – 713209.	Probing Magnetism in Iron Embedded MoTe2: A First-Principles Study
10	GARIMA AHUJA	Theoretical Sciences Unit, JNCASR Bengaluru, India	Engineering two dimensional electron and hole gases at Si/Si1−xGex heterostructure interfaces: Insights from DFT calculations
11	Gauswami Apeksha Shaileshgir	Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, India-390002.	Chiral Split Magnon in Altermagnet β-MnO2: A First-principles Study
12	Akhilesh kumar Gupta	Department of Physics,Maharaja Sayaji University of Baroda, Vadodara	Plant-derived Medicinal Biomolecules in an Aqueous Solution: A Quantum Mechanical Prediction for Efficacy Parameters
13	Anirban Roy	Department of Physics, University of Calcutta, 92 A. P. C. Road, Kolkata – 700009, India	Exploring Multifunctional Prospects of Metal-free Group-IV Carbide Quantum Dots and Their Single Layer Heterojunctions
14	Anoop Raj	Department of Physics, IIT Bombay, Mumbai - 400076	Phonon-assisted control of magnonic and electronic band splittings
15	ARUL RAJ NATARAJAN	Department of Physics, Indian Institute of Technology Hyderabad	Exploring Energy Materials from First Principles Study
16	Asfakujjaman	Department of Physics, University of Calcutta, , 92, A.P.C. Road, Kolkata 700009, India	A novel phase of germagraphene — Quasi-direct bandgap and anisotropic carrier mobility with potential optoelectronic response
17	Ashwath Subrahmanya P	Department of Physics, National Institute of Technology, Surathkal, Karnataka.	FIRST PRINCIPLES STUDY OF MULTIGAP SUPERCONDUCTIVITY IN V3Si USING MIGDAL – ELIASHBERG THEORY
18	Babuji Dandigunta	Department of Physics, IIT Madras, Chennai-600036, India	A Computational Framework for Accurate Estimation of Theoretical Specific Capacity: A Case Study of α–Graphyne
19	Anupama S	Physics Department, IISER Pune	High-temperature magnetism and strong spin-lattice coupling in two-dimensional CrTe2
20	BINOY KUMAR MAHATO	DEPARTMENT OF PHYSICS, BANARAS HINDU UNIVERSITY, VARANASI - 221005, INDIA	STATISTICAL PROPERTIES OF CONFINED SYSTEM

21	Bishal Das	Department of Physics, Indian Institute of Technology Bombay, Powai, Mumbai 400076, Maharashtra, India	Altermagnetism in Weyl semimetal GdAlSi
22	BUVANESWARAN S	SRM Institute of Science and Technology	Design of ferroelectric double perovskite oxides as photovoltaic materials
23	Debarghya Dutta	Centre for Research in Nanotechnology and Science, IIT Bombay, Powai, Mumbai 400076	Electronic and magnetic properties of Sr2TiFeO6 implementing ab initio density functional theory
24	Richa Sharma	National Institute of Technology Goa, India, 403703	Comparative Investigation of PdFeGa alloy using DFT and DFT+U for Multifunctional Applications
25	Riddhi D. Sainda	Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, India.	The enhaced efficient of two dimension polyaramide as glucose sensor
26	Rubee Swarnkar	Theoretical Sciences Unit, JNCASR, Jakkur, Banglore	Self-assembly of a Saddle Shaped Molecule on Metal Surface: Insights from First Principles
27	Sakshi Verma	Theroretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bengaluru 560064	Chemical tuning of metavalent bonding at the interfaces in chalcogenide superlattices
28	Sanat Nalini Paltasingh	Physics Department, School of Basic Sciences, Indian Institute of Technology Bhubaneswar, Khorda, Odisha, India, 752050	Interaction of Li/Na/K with Holey Graphyne-Nickel Sulfide Hetero System for Metal-Ion Battery Anode
29	Sanika S. Padelkar	Department of Physics, Indian Institute of Technology Bombay, Mumbai, Maharashtra, 400076, India and School of Chemistry, Monash University, Melbourne, Victoria, 3800, Australia.	Exciton-phonon coupling-mediated anomalous emission dynamics in a newly emerged twisted quasi-2D Piezoelectric Perovskite
30	Sarga P K	BITS PILANI KK BIRLA GOA CAMPUS -DEPARTMENT OF PHYSICS	MXene/Blue Phosphorene for Photocatalytic Overall Water Splitting Application.
31	Prosanta Sarkar	Department of Condensed Matter and Materials Physics, S. N. Bose National Centre for Basic Sciences, JD Block, Sector III, Salt Lake, Kolkata, West Bengal 700106, India	Electronic Structure of the Mixed Compounds, Ca_(1-x)La_xFe_(1-x)Mn_xO_3
32	R RAGHAVENDRA	Department of Chemical Engineering, Silver Oak Marg, Indian Institute of Science, CV Raman Avenue, Bangalore - 560012	A Physically Inspired Machine-Learnable Representation of Electronic Structure
33	Rahul Verma	Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Mumbai	Three dimensional higher-order van-Hove singularity in approximant quasicrystals
34	Rajdeep Boral	Research Institute for Sustainable Energy (RISE), TCG Centres for Research and Education in Science and Technology, Sector V, Kolkata, 700091, West Bengal, India	Accelerating diffusion analysis on halide solid electrolyte via on-the-fly machine learning force fields
35	Rashid Rafeek V Valappil	IISER Bhopal	Structural and Dynamic Changes in the High Pressure Phases of MAPbBr3 Unveiled by Machine Learning Force Field Simulations
36	Ritam Chakraborty	Theoretical Sciences Unit, JNCASR, Rachenahalli Lake Road, Jakkur, Bangalore 560064	Quadruply Fused Porphyrinoid Nanotapes on Surface: Insights from DFT
37	Ritwik Das	Indian Association for the Cultivation of Science	Topological Phase Transitions in Kagome Ferromagnets: The Role of Intrinsic Rashba Spin-Orbit Coupling
38	Robin Bajaj	Physics, Indian Institute of Science, Bangalore	Symmetries in zero and finite center of mass momenta excitons
39	Sadikul Alom	Institute of Advanced Study in Science and Technology, Guwahati, Assam, 781035, India	Berry Curvature-Induced Hall Effect in Mn_2PtSn Heusler Alloy: A First-Principles Study
40	Samim Reza	Department of Physics, SRM University AP, Guntur Andhra Pradesh	Identification of C3N/Silicene heterostructure as anode materials for Li-ion battery and its origin
41	Paromita Dutta	Indian Institute of Technology Bombay	Exploring Yb-based triangular lattice a potential candidate for quantum Spin liquids: HYbO2
42	Tanna Hemangkumar Pravinkumar	Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, India-390002.	Atomically Injected Ni-Atom over Graphene and Analogous Substrates for Hydrogen Evolution Reaction: A DFT Study
43	Deepak Upadhyay	Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda	Compression-Induced Comproportionation in Palladium Trifluoride

44	Bhautik Dhori	Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat 390002, India.	Coexistence of spin valley coupled Dirac semimetal and robust quantum spin Hall state in halogenated BiAs film
45	Zarna D. Ponkiya	Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, India-390002	Machine Learning Force Field-Accelerated Prediction and Modulation of Lattice Thermal Conductivity in 2D TMDs
46	Tukadiya Namrata A.	Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda	$RbGeBr_3$ Perovskite Solar Cells: Explored via DFT, Machine Learning and SCAPS-1D studies
47	Subrahmanyam Sappati	Gdansk University of Technology	DFT Perspective on Reactive Glass-Metal Interactions Enables Surface Modification of Gold Nano-Islands
48	Pankaj Gupta	IISER Pune	Enhanced thermoelectric properties of Zinc-Indium co-doped Sn1.03Te

DAY 2: May 20, 2025

Poster No:	Name	Affiliation	Title
1	Roshme Prakash	Department of Physics, Anna University, Chennai, Tamil Nadu, India, 600025.	Theoretical Investigation of Half-Metallic Ferromagnetism, Thermoelectric, and Optical Properties in Novel Half-Heusler RbXSb (X = V, Nb, and Ta) Alloys
2	Sadhana Barman	Department of Physics, Assam University, Silchar, Assam, 788011, India	Development of machine learned interatomic potential for thermal transport
3	ANKOSH DADARAM DESHMUKH	Department of Physics; Department of Scientific Computing Modeling and Simulation, Savitribai Phule Pune University Pune	A comparative study of a-TiO2 bulk and its Ni-modified (101) surface for photocatalytic applications
4	Supriya Ghosal	Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore 560064, India	Half-Heuslers to Double Half-Heusler: A potential route towards improved thermoelectric performance
5	Brajesh Rajesh Bhagat	Research Institute for Sustainable Energy, TCG-CREST, Salt Lake, Kolkata 700091, India	Investigation of the active Cu sites for CO2 reduction on 2D CuSiO3
6	Basavaraja G	Department of Physics, IISER Pune	Controllable Switching between Axion and Quantum Anomalous Hall States in CrI3/MnBi2Te4/CrI3 Heterostructures.
7	Bhakti Mangesh Kshirsagar	Department of Scientific Computing, Modeling and Simulation, Department of Physics, Savitribai Phule Pune University, Ganeshkhind, Pune, 411007	CsFeX3 (X= F, Cl, Br, I) Promising Materials for Spintronics and Infrared Optoelectronics
8	Laxman Tatikondewar	Department of Physics, Savitribai Phule Pune University, Pune -411007.	Are ultra thin transition metal dichalcogenides based excitonic solar cells exceptional ?
9	Pattanshetti Suman Panchamrut	Department of Physics, Savitribai Phule Pune University, Pune, India	Melting of harder-than-diamond lonsdaleite using machine learned potential
10	Pallavi Vyankuram Chame	Department of Chemistry, Indian Institute of Science Education and Research, Pune	Water dissociation on α-Titanium(0001): Insights into role of water vapour on early stages of high temperature oxidation of Titanium
11	Tanuja Joshi	JNCASR	Orientational Dependence of Spin Crossover Properties
12	Ashwini Verma	Physical and Material Chemistry division, CSIR-NCL Pune	Machine Learning - Driven Design and Synthesis of Materials for Solid-State Hydrogen Storage
13	Ashutosh Anand	Department of Physics, Indian Institute of Science Education and Research, Pune	Magnetic Phase Transition in LaVO3 thin films
14	Abhinav Prashant Gotmare	Manipal Centre for Natural Sciences, Manipal Academy of Higher Education, Eshwar Nagar, Manipal, Karnataka, India - 576104	Theoretical Investigation on the Magnetic and Spintronic behavior of 2D MXenes
15	Abhishek Bhattacharjee	School Of Physical Science, National Institure Of Science Education and Research	Orbital Free Density Functional Theory Applied On Solids And Finite Systems
16	aishwaryo ghosh	S N Bose National Centre for Basic Sciences, Dept of Condensed matter and materials physics, Salt Lake, JD Block, Sector 3, Bidhannagar, Kolkata, West Bengal 700106	Application of machine learning for solving materials science problems
17	Gayathri Palanichamy	Department of Physics and Nanotechnology, SRM University, Kattankulathur, Tamil Nadu, India.	Machine learning insights into Polarization and Magnetization switching dynamics in Hybrid Improper Ferroelectric Double Perovskites Oxides

18	Geetimallika Das	Department of Physics, Dibrugarh University, Dibrugarh Assam, 786004	Thermoelectric Performance of LiCaB Half-Heusler Alloys in Presence of Aliovalent Doping and Co-doping
19	Ishita Shitut	Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore	Stochastic G0W0 study on silicon nanocrystals
20	Jampala Pasyanthi	Department of Chemical Engineering, Indian Institute of Science (IISc), Bengaluru, Karnataka.	Developing fully ab initio classical force fields for 2D materials
21	Joyeta Saha	National Institute of Science Education and Research,Bhubaneswar. School of Physica; sciences.	Spatial distribution of Mayer bond order in periodic systems
22	Jyoti	Department of Physics, Indian Institute of Technology Kanpur	Enhanced Thermoelectric Performance of BaCuGdTe3 due to Strong Acoustic Phonon Suppression
23	Jyoti Bharti	Department of Chemistry , Indian Institute of Technology Delhi	Ligand-Driven Hot-Carrier Dynamics in Metal-Rich CdSe Quantum Dots: Insights from First-Principles and Nonadiabatic Molecular Dynamics
24	Khushboo	Department of Chemistry, IIT Madras	Hot Electron Transfer from Nanoparticle to PFAS Systems: A Size-Dependent Study
25	Muskan	Manipal Centre for Natural Sciences, Manipal Academy of Higher Education, Manipal 576104, Karnataka, India	Saturation of Magnetic Exchange Coupling with Increasing Cumulene Coupler Length in Diarylmethyl Diradicals
26	Namana V	Physics Department, Indian Institute of Science, Bengaluru	Ab-inito study of biexcitons using exciton product basis
27	PARVATHY S CHANDRAN	Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, Tamilnadu, India, 600036	Adsorbate-Adsorbate Interaction Model-based Prediction of Oxygen Coverage on Molybdenum Carbide Catalysts and Work Function Correlations
28	Renna Shakir	Department of Science and Humanities, Rajiv Gandhi Institute of Petroleum Technology (RGIPT), JAIS, Amethi, U.P	Exploring Metal-Doped C_2N Catalysts for CO_2 Reduction to C_2 Products via an Alternative C-C Coupling Pathway.
29	Debendra Meher	Chemistry and Physics Of Materials Unit (CPMU), Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR)	Machine Learning Potential Based Study of Borate Glasses
30	Deep Mondal	Department of Physics, University of Calcutta	Intriguing topological signatures in novel Dumbbell C3NX (X = C, Si, Ge) and its quasi-1D derivatives
31	Deepak Kumar Singh	Department of Physics, Institute of Science, Banaras Hindu University, Varanasi 221005, India	Machine learning Eigen-values, Eigen-functions and variational parameters
32	E V Charan Reddy	Department of Chemical Engineering, Indian Institute of Technology Bombay, Powai, Mumbai, Maharashtra 400076, India.	Mechanistic Insights into the Early Stages of Copper Oxidation: The Role of O-O Repulsion and Substrate-mediated Effects
33	Gurshidali Palakal	Theoretical Sciences Unit (TSU), Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR)	Material-specific investigations of strongly correlated electron systems through DFT+DMFT
34	Himanshu Murari	Department of Physics, Indian Institute of Technology Guwahati, Assam	Acoustic phonon restricted four-phonon interactions: Impact on lattice thermal conductivity in 2D h-NbN
35	Himanshu Sharma	Department of Physics, IIT Bombay	Optimising the electronic transport of Cu-based quaternary chalcogenide through first-principles study
36	Jay Panchal	Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara-390002, Gujarat, India.	Six-Fold Degenerate Phonons in the M3Sn (M = V, Nb): A density functional theory calculations
37	Jisvin Sam	Department of Physics, Indian Institute of Science Education and Research (IISER) Tirupati, Tirupati-517619, Andhra Pradesh India	Superconductivity and CDW phases in Ca intercalated bi-Layer silicene
38	Jyotirmoy Sarkar	Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Rachenahalli Lake Rd, Jakkur, Bengaluru, Karnataka 560064	An Effective Spin Hamiltonian: Renormalization by Vibration
39	K. Nithish Sriram	Research Scholar, Department of Theoretical Physics, School of Physics, Madurai Kamaraj University, Madurai - 625 021	Intermediate band formation and delocalization in second-row transition metal (Y, Zr, Nb, and Mo) doped Cu2O for photovoltaic applications: GGA+U study
40	Kartick Ramakrishnan	Department of Computation and Data Science, Indian Institute of Science Bangalore	PAW-DFT-FE: A fast and accurate real-space finite-element based method for large-scale ab-initio material modelling
41	Kaushik Santoshkumar Jayprakash	Department of Physics, Faculty of Science, The M S University of Baroda, Sayajigunj, Vadodara , Gujarat	Toxic Gas Sensing Mechanisms on 2D TMD Heterostructures: A First-Principles Approach.

42	Kunal Dutta	Indian Association for the Cultivation of Science, School of Physical Sciences, 2A and 2B Raja S.C. Mullick Road, Jadavpur, Kolkata 700 032, India	Symmetry induced novel spin textures in non-centrosymmetric systems
43	Lokesh Yadav	Department of Physics, Indian Institute of Technology Indore, Khandwa Road, Simrol, Indore-453552, India.	Exploring and Elucidating the CO2 Reduction Mechanisms on the Surface of Two-Dimensional Nitrogen-Vacancy (VN) Hexagonal Boron Nitride.
44	Mayank Sharma	Theoretical Science Unit (TSU), Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR)	Computational study of oxide-based spinel material for the application as cathode in Energy storage
45	Moinak Ghosh	Center for High-Performance Computing, Indian Institute of Science Education and Research Thiruvananthapuram, Maruthamala PO, Vithura, Thiruvananthapuram, Kerala 695551, India	Trends of magnetic interactions in transition-metal trilayers under electric-fields
46	Nidheesh Virakante	Department of Mechanical Engineering, IIT Bombay, Mumbai-400076	Effect of higher-order processes on the first-principles driven phonon thermal transport in ThO2
47	Pranjal Panwar	IISER Pune	Understanding the local electronic properties of ZrTe2 and ZrSeTe
48	Sagnik Chatterjee	IISER Pune	Brightening of momentum dark exciton via tensile strain induced valley convergence in WS2 monolayer

DAY 3: May 21, 2025

Poster No:	Name	Affiliation	Title
1	Nikhil Kodali	Department of Computational and Data Sciences, Indian Institute of Science Bengaluru,CV Raman Rd, Bengaluru, Karnataka 560012	Finite-element methods for noncollinear magnetism and spin-orbit coupling in real-space pseudopotential density functional theory
2	Nikhil Malviya	Department of Mechanical Engineering, Indian Institute of Science Bangalore	Phonon dynamics in ultrahigh thermal conductivity materials: accelerating the solution of first principles based Boltzmann transport equation
3	Nikhil Singh	Department of Chemistry, Indian Institute of Technology, Delhi, Hauz Khas, New Delhi 110016, India	High-throughput and data-driven search for stable optoelectronic AMSe3 materials
4	Pabitra Kumar Nayak	Department of Chemistry, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, India	Data-Driven Design of Electroactive Spacer Molecules to Tune Charge Carrier Dynamics in Layered Halide Perovskite Heterostructures
5	Paras Patel	Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara-390002, Gujarat, India	Structural Evolution of FeCl2 under High Pressure: A First-Principles Investigation
6	Prasann Kshatriya	Department of Physics, Sardar Vallabhbhai National Institute of Technology, Ichchanath Surat-Dumas Road, Keval Chowk, Surat, Gujarat 395007	Electrical and Optical Properties of BSe and Twisted Bi-Layer Graphene Heterostructure using DFT First principles Calculation
7	Pritam Ghosh	Materials Engineering, Indian Institute of Science, Bangalore	Metal Oxide-Based Hydrogen Sensors Beyond the Adsorbed-Oxygen Model: A Pt–ZnO Case Study
8	Pritish Joshi	Research Institute for Sustainable Energy (RISE), TCG Centres for Research and Education in Science and Technology, Sector V, Kolkata, 700091	Inverse design of cathode materials for metal-ion batteries using Variational Auto-Encoder neural network architecture
9	Shahla Karimpanakkal	Department of Chemical Engineering, Indian Institute of Technology Bombay, Powai, Mumbai, Maharashtra 400076, India	CO2 Hydrogenation on Orthorhombic Molybdenum Carbide: A Computational Study using DFT and ReaxFF
10	Shreya Chatterjee	Department of Chemistry, Indian Institute of Science Education and Research Bhopal, Bhopal, MP, 462 066, India.	Substituted Thiocoumarins Under Solvation and Confinement: A First-Principles Approach to Photophysics and Photochemistry
11	Srishti Bhardwaj	Department of Physics, Indian Instiute of Technology, Roorkee, Uttarakhand, India (247667)	Rare-earth halide based two-dimensional multiferroics
12	Sulagna Ghosh	Department - Physical Sciences; Institute - Variable Energy Cyclotron Centre, Bidhannagar, Kolkata - 700064, India	A theoretical insight on H2 adsorption over two-dimensional materials

13	Swati Shaw	Physics Department, IIT Guwahati, Guwahati-781039, Assam, India.	Comparative Study of Photocatalytic Water Splitting and CO 2 Conversion Over Infrared and Visible Active Janus MXenes
14	Sweta Ghosh	School of Physical Sciences at IIT Goa	Electric field induced Rashba state in topological layered intermetallics
15	Tamilmani S	Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai - 600036	Mechanistic Insights and Design Principles for Efficient NH_3-SCR Catalysts: A DFT Study on Fe_2O_3 and NiO Systems
16	Alpa Dashora	Department of Physics, Faculty of Science, The M.S. University of Baroda, Sayajigunj, Vadodara 390002 (Guj)	Unveiling heterogeneously active HER sites by surface reconstruction via termination groups in MXenes
17	Anita Gemmy Francis	JNCASR	Quasiparamagnetic ground state in hyperhoneycomb lattice compound NaYbW2O8
18	Mayuri Bora	Department of Physics, IIT Guwahati, Amingaon, North Guwahati, Guwahti 781039, Assam, India	Electrically tunable valleytronics in 2D ferrovalley/ferroelectric heterostructure
19	Sanuja Kumar Khuntia	PhD Scholar, Department of Condensed Matter and Materials Physics, S. N. Bose National Centre for Basic Science, Kolkata, India, 700106	What drives the distortions in 2D hybrid perovskites?
20	Saptarshi Ghosh Dastider	Department of Physics and Astrophysics, University of Delhi,. New Delhi, India, 110007	Bimetallic Molecular Model Inspired Designing of M–Zn–N–C (M = Fe, Co, Ni, Cu) type Catalysts for Enhanced HER and OER Performance.
21	Sarvesh Shamsundar Medhekar	Department of Mechanical Engineering, Indian Institute of Science, Bangalore, 560012, India	Coupled electron-phonon dynamics in polar semiconductors: A first-principles Boltzmann transport approach
22	Vaibhav Walve	IISER Pune	Unveiling different structural orderings in Fe5-xGeTe2
23	Saurav Patel	Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, India-390002	Non-trivial Topology, Hyperferroelectricity and Giant Rashba Spin-splitting in Non-centrosymmetric LiZnAs Compound
24	Shantanu Semwal	Department of Physics, Indian Institute of Technology Kanpur, UP 208016, India	Concerted rattler dynamics induce glass-like thermal conductivity in crystalline TlAgTe
25	Shovan Gayen	Ph. D Scholar, Bennett University, Greater Noida, UP-201310, India	Magnetism in a two-dimensional honeycomb antiferromagnet BaNi2(XO4)2; (X=P, V & As): A combined DFT+U and Monte-Carlo simulations
26	Sk. Soyeb Ali	Ph.D Scholar, Bennett University, Greater Noida, UP-201310, India	Strain induced electronic and magnetic transition in S=3/2 ferromagnetic spin chain compound SbCrSe3
27	Sougata Saha	Theoretical Sciences Unit,JNCASR, Jakkur, Bangalore-560 064	Metal-Doped Fullerene: Promising Electrocatalysts for Hydrogen and Oxygen Evolution Reactions
28	Soumyadeep Bhattachrayya	School of Physical Sciences, Indian Institute of Technology Goa, Farmagudi (at GEC campus), Goa - 403401	Crucial role of Fe-Fe magnetic interactions in layered triangular antiferromagnet in dictating Li-ion cathode material efficiency
29	Sourav Ghosh	Department of Physics, SRM University AP, Mangalagiri -Mandal, Neeru Konda, Amaravati, Andhra Pradesh 522502	M-NxB SAC Catalysts with CO gas as Reactant Selective Towards C2 Product
30	Sourav Mal	Department of Physics, Harish-Chandra Research Institute, Chhatnag Road, Jhunsi, Prayagraj, 211019, India	Generative AI Model for Designing Magnetic Materials
31	Srinibas Nandi	Phd Student, Department of Computational and Data Sciences, Indian Institute of Science, Bengaluru, Karnataka, 560012	A computational methodology for kinetic energy density dependent meta-GGA functionals in finite-element based DFT calculations with accelerated self-consistent field iterations
32	Subas Rana	Physics Department, IIT Kanpur, Kalyanpur, 208016, Uttar Pradesh	Semi-universal Solution of Thomas-Fermi Equation for Jellium Spheres
33	suhail ahmad bhat	Department of Physics, School of Natural Sciences, Shiv Nadar Institution of Eminence, Dadri, Greater Noida, U.P. - 201314	Exploring Titanium-Doped Vn+1CnO2 MXenes as Efficient Urea Adsorbents for Wearable Artificial Kidneys
34	Suhas Adiga	Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru	Accelerating the Search for Superconductors Using Machine Learning
35	Sujith N S	School of Physical Sciences, NISER Bhubaneswar, Jatni, Odisha-752050, India	Large electro-mechanical actuation in hydrogenated Xenes leading to topological transition
36	AATHIRA NAIR	PHYSICAL AND MATERIALS CHEMISTRY, CSIR NATIONAL CHEMICAL LABORATORY PUNE, 411008	EXPLORING THE FOUNDATIONS: PREREQUISITES FOR EPOXIDATION
37	Khorsed Alam	Chemistry Department, Bar-Ilan University, Ramat Gan, Israel 5290002	Monte Carlo Simulated Annealing and Machine Learning Interatomic Potentials for High-Entropy Materials Design

38	Mohammad Ubaid	Department of Physics, Indian Institute of Technology Kanpur, Uttar Pradesh 208016, India	Data-driven Discovery of Novel High-performance Quaternary Chalcogenide Photovoltaics
39	Soumendra Kumar Das	Post Doctoral Fellow	Impact of oxygen and ozone exposer on the reaction kinetics of two-dimensional C2N monolayer: A First Principles Study.
40	Surajit Adhikari	Department of Physics, Indian Institute of Technology, Bombay, Powai, Mumbai 400076, India	Inorganic Antiperovskite Derivatives: Next-Gen Materials for Optoelectronics
41	Tushar Kanti Ghosh	Department of Chemistry, Purdue University	Manipulating van der Waals Interaction with Strong Light-matter Coupling
42	Piyush Ranjan Maharana	Physical and Materials Chemistry, CSIR-National Chemical Laboratory, Homi Bhabha Road , Pune - 411 008, India.	Retrieval augmented generation for building datasets from scientific literature
43	Sutapa Chattopadhyay	Department of Physics, Savitribai Phule Pune University	Topological properties of CdX (X = S,Se,Te) nanoribbons
44	Krushna Rajendra Zoting	Department of Physics, Fergusson College (Autonomous), Pune	Exploring the Potential of Cadmium Sulphide (CdS) via First-Principles Calculations: Electronic, Optical, and Thermoelectric Perspectives
45	Sarika Lohkna	IISER Pune	AB INITIO STUDY OF CO2 CONVERSION ON MOS2 MONOLAYERS WITH S VACANCIES: 2H V/S 1T V/S 1T' PHASE
46	Sudipta Majumder	IISER Pune	Role of lateral Di-Sulfur Defects in Achieving High Mobility in MoS2 Monolayers