AAPALI PSI-K 2025

International Conference on Electronic-Structure Theory and Applications

May 19 – 21, 2025

Venue: Lecture Hall Complex, IISER Pune Campus

Day 1: May 19, 2025

8:00 - 9:00	Registration, Lecture Hall Complex (LHC)
9:00 - 9:30	Inauguration, C. V. Raman Auditorium, LHC
9:30 - 10:00	Tea Break

	Parallel Session I (LHC 101)		Parallel Session II (LHC 201)		Parallel Session III (LHC 103)	
	Methods 1 : Spectroscopy & Excited States (Chair: Shouvik Datta)		**Catalysis 1** (Chair: Ranjit Thapa)		**Magnetism 1 -SOC** (Chair: Sunil Nair)	
10:00 - 10:25	Lucia Reining	Fingerprints of excitonic effects in valence electron spectroscopies	Sharan Shetty	Computational Insights in Heterogenous Catalysis: An Industrial Perspective	Subhradip Ghosh	Rashba and Zeeman effects in non-magnetic MXene
10:25 - 10:50	Claudia Draxl	Theoretical Spectroscopy Including Electron-Phonon and Exciton-Phonon Coupling	P Ravindran	Graphene Based Photocaltalysts for Green Hydrogen Production	Souvik Paul	Magnetic skyrmions on the noncollinear ground state
10:50 - 11:15	Manish Jain	Ab-initio multiparticle excitations in materials	Krishnakanta Mondal	Modelling of Transition Metal Based Catalyst for Hydrogenation of CO2 towards Fuel	Tanusri Saha Dasgupta	Interplay of SOC and Coulomb Interaction – Route to Unconventional

11:15 - 11:45	Tea Break

	Parallel Session I (LHC 101)		Parallel Session II (LHC 201)		Parallel Session III (LHC 103)	
	Methods 2: Spectroscopy & Excited States (Chair: Nirmalya Ballav)		**Catalysis 2** (Chair: Sharan Shetty)		**Magnetism 2 - SOC** (Chair: Ashish Arora)	
11:45 - 12:10	Hannes Jonsson	Variational Calculations of Excited Electronic States by Converging on Saddle Points on the Electronic Energy Surface	Bidisa Das	DFT studies of Fe oxyhydroxide Nanostructures in Water: Structure and OER Activity	Debjani Karmakar	Complex Chiral Magnetism in Quasi-2D Fe4GeTe2

12:10 - 12:35	Saswata Bhattacharya	Role of Dimensionality on Excitonic Properties of BiSeI from Many-body Perturbative Approaches	Ranjit Thapa	Electronic descriptors for metal center catalysts to define C2 product selectivity during CO2ER	Sukanya Ghosh	Intriguing Tale of van-der-Waals Magnets: Interplay of Unusual Structural Reconstruction, Exchange Mechanism and Electron Correlation
12:35 - 13:00	Saswata Roy	Divergences within TDDFT	Utpal Sarkar	Structure and reactivity of fullerenes and their derivatives	Cyrille Barreteau	Modelling spin-orbitronics effects at inorganic interfaces and through chiral molecules

13:00 - 14:40	Lunch at The Dining Hall Complex (First Floor)

	Parallel Session I (LHC 101)		**Parallel Session II (LHC 201)**		**Parallel Session III (LHC 103)**	
	Methods 3: Codes (Chair: Swapan K Pati)		**Thermal Properties 1** (Chair: Shobhana Narasimhan)		**Magnetism 3 - Altermagnets** (Chair: Arijit Bhattacharyay)	
14:40 - 15:05	Ryoji Sahara	Electronic structure in light-element-doped TiO2 by all-electron GW calculation using TOMBO code	Hena Das	Thermal expansion in cross-coupled order parameter oxides	Birabar Ranjit Kumar Nanda	Electronic Structure of Altermagnetic Materials: A Chemical Bonding Perspective
15:05 - 15:30	Phani Motamarri	Fast and accurate finite-element based methods for DFT calculations within the projector-augmented wave formalism in the exascale era	Narayan Prasad Adhikari	Exploration of some efficient high temperature thermoelectric materials: a focus on half Heuslers	Nirmal Ganguli	Altermagnetism from nonsymmorphic symmetry
15:30 - 15:55	Malaya K Nayak	Development and implementation of new features in fully-relativistic DIRAC program package	Bulumoni Kalita	Improved Thermoelectric Properties of Doped and Strained XCaB (X-Li, Na, K) Alloys	Awadhesh Narayan	Interplay of altermagnetism and pressure

16:00 - 17:15	Poster session + High Tea

17:30 - 19:00	Birthday celebration of Prof. Dilip G Kanhere (C. V. Raman Auditorium, LHC)

19:30 - 21:00	Dinner at The Dining Hall Complex (First Floor)

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Day 2: May 20, 2025

	Parallel Session I (LHC 101)		Parallel Session 2 (LHC 201)		Parallel Session 3 (LHC 103)	
	High throughput & ML (Chair: D. G. Kanhere)		**Charge and Defects** (Chair: Kavita Joshi)		**Quantum Materials 1: Hall Effects and van Hove Singularities** (Chair: Sreejith G. J.)	
9:00 - 9:25	Aron Walsh	Rapid Exploration of Crystal Chemical Space	Nisanth N Nair	Excess Electron in Water	Bheemalingam Chittari	Topological Quantum Hall Phases in Twisted Bilayer Graphene and Orbital Hall Phases in Rhombohedral Multilayer Graphene
9:25 - 9:50	Laalitha S. I. Liyanage	High Throughput Computational Materials Design	Tanmoy Paul	Ab initio study of point defects in halide solid electrolytes	Munima B. Sahariah	Anomalous Hall Effect in Pt-based Heusler alloy
9:50 - 10:15					Bahadur Singh	High-Order van Hove Singularities as a Route to Emergent Quantum States
10:15 - 10:45	Tea Break					
	Parallel Session I (LHC 101)		**Parallel Session 2 (LHC 201)**		**Parallel Session 3 (LHC 103)**		**Parallel Session 4 (LHC 203)**	
	Machine Learning 2 (Chair: D. G. Kanhere)		**Thermal properties 2 - Transport** (Chair: Hena Das)		**Quantum Materials 2 : Topology** (Chair: B R K Nanda)		**Batteries** (Chair: Arun Venkatnathan)	
10:45 - 11:10	Jan Janssen	Ab-initio Temperature Concentration Phase Diagrams	Anees Pazhedath	Unlocking the Thermal Transport in Disordered Solids: A Computational Approach using Wigner Formulation	Gour Prasad Das	The emerging world of topological semimetals	Priya Johari	Computational Design of High-Performance Electrode Materials for Next-Generation Li-ion and Na-Ion Batteries
11:10 - 11:35	Stefano de Gironcoli	Toward General-Purpose Machine Learning Interatomic Potentials	Ankit Jain	Accelerating thermal conductivity prediction through machine-learning	Banasree Sadhukhan	Mapping from fermionic to bosonic topology in incommensurate spin spiral of kagome-lattice YMn6Sn6	Mudit Dixit	Designing Cathode Materials for Li-Ion and Na-Ion Batteries Using Advanced Computational Methods
11:35 - 12:00	Amreen Bano	Machine Learning-Assisted Design and DFT Validation of High Entropy Na-Deficient Cathode Materials	Navaneeth Krishna Ravichandran	Thermal transport in Semiconductors Studied Using a Physics- and Data-Driven Solution of the Peierls-Boltzmann Equation	V Kanchana	Unveiling the Device Applications of Emerging Topological Materials Topological	W. Wasanthi P De Silva	Revolutionizing Energy Storage: The Role of DFT in Battery Material Innovation
12:00 - 12:25	Sai Gautam Gopalakrishnan	Machine Learning Guided Exploration of Amorphous Electrodes and Electrolytes	Koushik Pal	Indispensable roles of anharmonic renormalization, high-order scattering and wave-like tunnelling of phonons in ultralow thermal conductivity semiconductors	Poorva Singh	Unveiling Novel Topological Phases: Theoretical Insights and Predictions		
12:30 - 14:30	Lunch at The Dining Hall Complex (First Floor)							
	Parallel Session I (LHC 101)		**Parallel Session 2 (LHC 201)**		**Parallel Session 3 (LHC 103)**		**Parallel Session 4 (LHC 203)**	
	Chemical thermodynamics (Chair: Subhradip Ghosh)		**Methods 4** (Chair: Nirmal Ganguli)		**Magnetism 4** (Chair: G. P Das)		**2D Materials 1** (Chair: Aparna Deshpande)	
14:30 - 14:55	Anuj Goyal	Predicting thermochemical equilibria with interacting defects: Sr(1-x)Ce(x)MnO(3-δ) alloys for water splitting	NS Vidhyadhiraja	DFT+DMFT modeling of strongly correlated electron systems	Priya Mahadevan	Examining the ground state of the Slater insulator NaOsO3	Abir De Sarkar	DFT perspectives on piezoelectricity and spin-orbitronics in selected functional 2D materials

14:55 - 15:20	Swastika Chatterjee	Isotopes as proxies to understand earth system processes: The role of first-principles calculations	Joydeep Bhattacharjee	Distribution of Charge Centers in Matter from Geometric Phases of Electrons	Sayantika Bhowal	Hidden Magnetic Order and Engineering of Non-Relativistic Spin Splitting	Santanu Mahapatra	Atomistic Insight to Non-Volatile Restive Switching in 2D Materials
	Parallel Session I (LHC 101)		**Parallel Session 2 (LHC 201)**		**Parallel Session 3 (LHC 103)**		**Parallel Session 4 (LHC 203)**	
	MOFs and Alloys (Chair: Subhradip Ghosh)		**Semiconductors** (Chair: Amrita Bhattacharya)		**Magnetism 5** (Chair: G. P Das)		**2D Materials 2** (Chair: Aparna Deshpande)	
15:35-15:55	Nurapati Pantha	Metal Organic Frameworks for the detection and storage of small gases	Vaishali Shah	First principles studies on green alternatives to popular piezoelectric and photocatalytic ceramics	Anita Halder	Van der Waals Magnets: Exploring Near-Half-Metallicity and Spin-Polarized Tunneling for Future Spintronic Applications	Appalakondaiah Samudrala	Role of Interlayer coupling on electronic and optical properties of MX2 (M= Mo / W, X= S / Se) Heterobilayers
15:55 - 16:20	Srinivasu Kancharlapalli	Computational Studies to Explore Metal Organic Frameworks for Energy Related Applications	Vijay Kumar	Ab initio studies of halide perovskites and β-W	Suranjan Shil	Magnetic Property Calculations with DFT: When GGA Functionals Outperform Hybrid Functionals	Varadharajan Srinivasan	Plasmon Induced Energy and Charge Transfer Dynamics in Metallic Nanoparticle-MoSe2 Nanoflake Heterostructures
16:20 - 16:45	N S Harsha Gunda	First-Principles Insights into Interstitial–Substitutional Interactions in Titanium Alloys	Swapan K Pati	Computational Modeling of Semiconducting Materials for Their Applications in Transport Properties	Indra Dasgupta	Spin-Orbit Coupling and Emergent Topological Phases in two Dimensional Ferromagnets		
16:50 - 18:05	Poster Session 2 + High Tea							
19:00 onwards	**Banquet Dinner at 2BHK Diner and Key Club** **The Mills (Behind Sheraton Grand Pune Station), Pune, Maharashtra 411001**							

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Day 3: May 21, 2025

	Parallel Session I (LHC 101)		Parallel Session 2 (LHC 201)		Parallel Session 3 (LHC 103)		Parallel Session 4 (LHC 203)	
	Machine Learning 3 (Chair: Arnab Mukherjee)		**Catalysis 3 & Energy** (Chair: Varadharajan Srinivasan)		**Magnetism 6 and Quantum Materials 3** (Chair: Awadhesh Narayan)		**Methods - Functionals** (Chair: Indra Dasgupta)	
9:00-9:25	Prasenjit Sen	Machine Learning aided efficient screening and inverse design of materials using generative models	Prafulla K Jha	Engineering 2D Monolayers for Optimized Hydrogen Evolution: A Computational Perspective	Amrita Bhattacharya	In search of rare earth free permanent magnets	Leeor Kronik	Solving the band gap and optical absorption problems of density functional theory
9:25 - 9:50	Ananth Govindrajan	Machine Learnable Representations of Materials, Molecules, and Reactions for Accelerating Materials and Mechanism Discovery	Jithin John Varghese	CO2 Reduction to Methanol: DFT Microkinetic Insights into Catalytic Structure-Activity Relations	Kartick Tarafder	The Complex Topological Order In Functional Materials	Manoj Harbola	Semi-universal solution of Thomas-Fermi equation for jellium spheres
9:50 - 10:15	Abhinav S. Raman	Artificial Intelligence-Enabled Molecular Simulations: Making Computers Learn Chemistry at Aqueous Oxide Interfaces	Aftab Alam	Biphenylene: A Promising Candidate for Renewable Energy Applications	Ganapathy Vaitheeswaran	Fermionic and Bosonic Topologies in Pyrite-Structured SiX_2 (X = P, As)	Prasanjit Samal	Towards Accurate Material Properties: New Computational Methodologies for Quantum Materials
10:15 - 10:40			Saroj Nayak	Computational Design of Functional Materials: From Super Capacitor to Green Hydrogen	Tilak Das	Magnetostrictronics: A bi-directional exchange of magnetic anisotropy and elastic energies	Rabeet Singh	Levy-Perdew-Sahni equation and its application to perform atomic calculations

10:40 - 11:55	Poster Session and Tea

11:55 -12:45	Dilip Kanhere: 50 years of computing: The Indian scene C. V. Raman Auditorium

12:45-14:15	Lunch at The Dining Hall Complex (First Floor)

	Parallel Session I (LHC 101)		Parallel Session 2 (LHC 201)		Parallel Session 3 (LHC 103)	
	Machine Learning 4 + Algorithms (Chair: Prasenjit Sen)		**Semiconductor Interfaces** (Chair: Angshuman Nag)		**Quantum Materials 4** (Chair: Aftab Alam)	
14:15-14:40	Sudarshan Vijay	Computing properties of charged molecules and surfaces using efficient periodic density functional theory implementation of Coulomb kernel truncation and machine learning interatomic potentials	Shobhana Narasimhan	Engineering Two-Dimensional Electron and Hole Gases at Semiconductor Heterostructure Interfaces	Swarup Kumar Panda	Competing Interactions, Spiral Order, and Emergent Spin Liquid Behaviour in Trigonal CaMn2P2
14:40-15:05	Anirban Mukherjee	Distributed QPU+GPU implementation of Tensor Factorized Hamiltonian Downfolding for electronic structure modelling	Dibyajyoti Ghosh	A Computational Insights into the Messy World of Quantum Dot Surfaces	Barun Ghosh	Quantum Geometry and Dynamical Axion in antiferromagnetic topological insulator $MnBi_2Te_4$
15:05-15:30			Paramita Ghosh	Epitaxial growth of thin film of germanium on 2×1 reconstructed silicon (001) surface: A kinetic Monte Carlo study	Sudipta Kanungo	Nonsymorphic symmtery enforced band topology

15:40-16:10	Closing Session C. V. Raman Auditorium

16:10 - 16:40	High Tea

19:30 - 21:00	Dinner at The Dining Hall Complex (First Floor)