Schedule for NAMMA Psi-k Workshop 2023

All Poster Sessions will be at AMRL Foyer and Library Quadrangle, JNCASR

Day 1: Monday, July 24 (JNCASR)

9:00-10:30 am	Review of the fundamentals of DFT (Manoj Harbola) AMRL Conference Hall
10:30-11:00 am	Coffee break AMRL Foyer
11:00-12:30 pm	Introduction to density functional perturbation theory (Umesh Waghmare) AMRL Conference Hall
12:30-2:00 pm	Lunch Conference Dining Hall
2:00-3:30 pm	Hands-on session on DFT ICC, College Building
3:30-4:00 pm	Coffee break Ground Floor, College Building
4:00-5:30 pm	Hands-on session on DFPT ICC, College Building
6:30-8:00 pm	Dinner (at JNCASR) Conference Dining Hall

Day 2: Tuesday, July 25 (JNCASR)

9:00-10:30 am	Fundamentals of AI/ML (Prasenjit Sen) AMRL Conference Hall
10:30-11:00 am	Coffee break AMRL Foyer
11:00-12:30 pm	Applications of ML to Materials Science (Sai Gautam Gopalakrishnan) AMRL Conference Hall
12:30-2:00 pm	Lunch Conference Dining Hall
2:00-3:30 pm	Hands-on session on basic AI/ML ICC, College Building
3:30-4:00 pm	Coffee break Ground Floor, College Building
4:00-5:30 pm	Hands-on session on neural networks ICC, College Building
6:30-8:00 pm	Dinner (at JNCASR) Conference Dining Hall

Day 3: Wednesday, July 26 (JNCASR)

9:00-9:30 am	Opening remarks (AMRL Conference Hall)		
9:30-11:00 am	**Session 1A (AI/ML-1)** AMRL Conference Hall Chair: Bidhan Chandra Garain	**Session 1B (Energy Materials-1)** Kanada Auditorium Chair: Prasad Matukumilli	**Session 1C (2D Materials-1)** Sheikh Saud Hall, SSL Chair: Arpan Das
	Tanusri Saha Dasgupta Machine Learning Approach of Design of New Materials with Targeted Properties	**Subhradip Ghosh** Computational modeling of electrochemical capacitance of Nitrogen doped $Ti_3C_2T_x$ supercapacitor electrode in acidic electrolyte	**Santanu Mahapatra** Unsupervised Learning Driven Discovery of 2D Charge-Density-Wave Materials
	Anirudh Natarajan Computational tools for the ab-initio design of high-temperature structural alloys	**Swapan K Pati** Computational Modeling of Materials for Energy Conversion	**Abir De Sarkar** DFT perspectives on valleytronics, piezoelectricity and spintronics in selected functional 2D materials

	Satadeep Bhattacharjee Unlocking materials properties: Exploring approaches from symbolic regression to deep learning	**G P Das** Computational design of materials for energy storage	**Priya Mahadevan** Why do twisted bilayers behave differently from their untwisted counterparts?
11:00-11:30 am	Coffee break (AMRL Foyer, SSL Foyer)		
11:30-1:00 pm	**Session 2A (Energy Materials-2)** AMRL Conference Hall Chair: Arijit Sinha	**Session 2B (Quantum Materials-1)** Kanada Auditorium Chair: Nikhil Avula	**Session 2C (Materials under pressure)** Sheikh Saud Hall, SSL Chair: Supriti Dutta
	Saroj Nayak Computational Design of Sustainable Materials: From Super Capacitor to Solar Energy	**Aparna Chakrabarti** Exploring the Prospect of Technological Applications of Quantum Materials using DFT	**G. Vaitheeswaran** Metallization of Solid Iodanil ($C_6I_4O_2$) under pressure
	Rajeev Ahuja Cancelled	**V Kanchana** Exploring Quantum Emergence: Unveiling the Phenomena and Properties of Quantum Materials	**Swastika Chatterjee** Detecting water deep inside the earth's mantle
	D D Sarma Putting a spin on battery electrodes - the importance of strong correlation physics	**Indra Dasgupta** Spin-Orbit Coupling Induced Emergent Phases in Quantum Materials	**Varadharajan Srinivasan** Probing the role of compression rates in the pressure-induced polymerization of crystalline acrylamide through ab initio molecular dynamics
1:00-2:00 pm	Lunch (Conference Dining Hall) Poster Session (AMRL Foyer, Library Quadrangle)		
2:00-3:30 pm	Poster Session (AMRL Foyer, Library Quadrangle)		
3:30-4:00 pm	Coffee break and Poster Session (AMRL Foyer, Library Quadrangle)		
4:00-6:00 pm	Celebration of Shobhana Narasimhan's 60th birthday (**Speakers/Faculty:** AMRL Conference Hall and **Students/post-docs:** Kanada Auditorium)		
6:30-9:30 pm	Dinner (at JNCASR) (**Speakers/Faculty:** Conference Dining Hall and **Students/post-docs:** Hostel 5th Block, Ground Floor		

Day 4: Thursday, July 27 (IISc – Physical Sciences Building)

9:00-10:30 am	**Session 3A (Methods-1)** Physics Auditorium Chair: Ishita Shitut	**Session 3B (Quantum Materials-2)** Lecture Hall 5 (New Annex) Chair: Sanat K Gogoi	**Session 3C (AI/ML-2)** Multimedia Room Chair: Dhondi Pradeep
	Stefano Battaglia Hybrid quantum-classical periodic embedding	**Awadhesh Narayan** Berry curvature dipole and non-linear Hall effect in two-dimensional materials	**Koushik Pal** Leveraging Data-driven approaches to accelerate Novel Materials Discovery
	Joydeep Bhattacharjee Estimation of quasi-particle band-gap and optical absorption threshold of large systems in a minimal tight-binding basis	**Bahadur Singh** Local structural motifs driven topological electronic states in quantum materials	**Balasubramanian S.** Machine Learning Models and Potentials for shear viscosity of fluids
	Rabeet Singh Confined two-electron atomic systems without using any cut-off factor in the wavefunction explicitly	**Prafulla K Jha** Exploring the Quantum Frontier: Topological Insulators and Their Extraordinary Properties.	**Kavita Joshi** Solid-state hydrogen storage: Decoding the path through machine learning

10:30-11:00 am	Coffee break (Next to Physics Auditorium)		
11:00-12:30 pm	**Session 4A (AI/ML-3)** Physics Auditorium Chair: Sucheta Swetlana	**Session 4B (Methods-2)** Lecture Hall 5 (New Annex) Chair: Kartick Ramakrishnan	**Session 4C (Thermal Properties)** Multimedia Room Chair: Anand Mohan Verma
	Prasenjit Sen Machine Learning aided exploration of materials space and inverse design of materials	**Manoj Harbola** Inversion problem in density functional theory	**Ankit Jain** Phonon thermal transport in low- and high-thermal conductivity solids
	Sai Gautam G Modelling complex configurational spaces with machine learned interatomic potentials	**Prasanjit Samal** Challenges ahead of ML-DFT: Additions within and beyond the Jacob's Ladder of DFT from Semilocal through Dielectric Dependent Hybrids	**Navaneeth Ravichandran** Controlling heat flow by manipulating phonons and their interactions: a bottom-up approach
	P Ravindran Machine learning driven DFT approach to understand and design new functional materials for energy technology	**Vikram Gavini** Towards Large-scale Quantum Accuracy Materials Simulations	**Aftab Alam** Thermoelectric Properties of Topological Semimetal $Cu_2ZnGeTe_4$: A New paradigm to Renewable Energy
12:30-2:00 pm	Lunch (Physics Conference Lunch Area)		
2:00-3:30 pm	**Session 5A (Chalcogenides and MXenes)** Physics Auditorium Chair: Garima Ahuja	**Session 5B (Magnetism-1)** Lecture Hall 5 (New Annex) Chair: Nikhil Kodali	**Session 5C (Catalysis-1)** Multimedia Room Chair: Ankit Kumar Verma
	Valerio Vitale Tuning the electronic structure of a twisted transition metal dichalcogenide heterotrilayer with a vertical electric field	**Biplab Sanyal** Complexities in electronic structure and magnetism of 2D Fe_nGeTe_2 (n=3, 4, 5) magnets	**Prasenjit Ghosh** C-vacancy Mediated Methane Activation and C-C Coupling on Titanium Carbide Surface
	Umesh Waghmare Metavalent Bonding Origins of Unusual Properties of Group IV Chalcogenides	**Munima B Sahariah** Stoichiometry dependent properties in Mn-based Heusler alloys: An ab initio study	**Jithin John Varghese** Computational spectroscopy and first principles microkinetic modelling in computational catalysis
	Arti Kashyap Magnetic MXene: A Machine learning model with small data	**Nirmal Ganguli** Asymmetry-Driven Spin-Splitting for Spintronics and Topological Quantum Technology	**Tej Choksi** On the Data-Driven Design of Stable, Active, Selective, and Cost-Effective Nanocatalysts for the Oxygen Reduction Reaction
3:30-4:00 pm	Coffee Break (Next to Physics Auditorium)		
4:00-5:30 pm	Panel Discussion (Physics Auditorium)		
6:30-9:30 pm	Conference Banquet (Comfort Inn Insys, Mathikere)		

Day 5: Friday, July 28 (IISc – Physical Sciences Building)

9:00-10:30 am	**Session 6A (Magnetism-2)** Physics Auditorium Chair: Nesta Benno Joseph	**Session 6B (Perovskites-1)** Lecture Hall 5 (New Annex) Chair: Arka Bandyopadhyay	**Session 6C (Methods-3)** Multimedia Room Chair: Shinjan Mandal
	Mukul Kabir Manipulating Magnetism in Two-Dimension	**Dibyajyoti Ghosh** Energy Materials: Atomic-scale Insights from ab initio modelling	**Nisanth Nair** Molecular dynamics simulations at the fourth rung of DFT functionals
	Souvik Paul New routes to control skyrmions in ultrathin transition-metal films	**Michele Kotiuga** A symmetry-based approach to identify structural prototypes and its application to perovskites	**Phani Motamarri** Fast and accurate real-space finite-element based methodologies for Projector-Augmented Wave (PAW) formalism in density functional theory calculations
	Debjani Karmakar Spin-dynamical ground-state: An answer to the inherent symmetry breaking in magnetic superconductors	**Sudip Chakraborty** Computational Roadmap of Hybrid Perovskites Materials: Insight from Rashba Effect and Piezochromism	**NS Vidhyadhiraja** Material-specific investigations of strongly correlated electron systems through DFT+DMFT
10:30-11:00 am	Coffee break (Next to Physics Auditorium)		
11:00-1:00 pm	**Session 7A (Energy Materials-3)** Physics Auditorium Chair: Tanmoy Paul	**Session 7B (Defects)** Lecture Hall 5 (New Annex) Chair: Manoj Dey	**Session 7C (Perovskites-2)** Multimedia Room Chair: Ritam Chakraborty
	Priya Johari Computationally Predicted Efficient Energy Materials	**Ayan Datta** Buckling and Defects in Two-Dimensional Atomically Thin Monolayers	**Ranjit Nanda** A theoretical framework to analyze and tailor electronic and optoelectronic properties of halide perovskites
	Mudit Dixit Designing Improved Cathode Materials for High-Capacity Sodium-Ion Batteries through Electronic Structure Tuning	**Bulumoni Kalita** Effect of Structural Point Defects on Electronic Properties of MgO Monolayers	**Amrita Bhattacharya** Exploring the thermodynamic stability and spin orbit driven Rashba splitting in Perovskite oxides
	Hemant Kumar Improving the Design of Solid-State Electrolytes with Machine Learning	**Ananth Govind Rajan** First-Principles Discovery of the Mechanisms Underlying the Synthesis of Nanoporous 2D Materials	**Ambesh Dixit** Designing Lead-free $Cs_2BB'X_6$ Double Perovskites for Energy Application(s): A Hybrid Computational Approach
	Ranjit Thapa Electronic Descriptor then Predictive model using QM/ML Approach then Experimental Validation	**Anuj Goyal** A computational framework to accelerate defect energy prediction and materials discovery for clean energy applications	**Chaitanya Sharma** Exploring the Formation and Evolution of Solid Electrolyte Interphase at Calcium Surfaces
1:00-1:10 pm	Closing Remarks (Physics Auditorium)		
1:10-2:30 pm	Speakers' Lunch (Main Guest House (MGH) IISc) + Participant Lunch (Physics Conference Lunch Area)		