

Schedule of International Conference on 60 Years of DFT: Advancements in Theory & Computation

School Schedule

Date and Time	Speaker	Title
22- July (School)		
9:00 AM to 9:30 AM	Inaugural Session	
9:30 AM to 11:00 AM	Manoj Harbola	Introduction to DFT
11:00 AM to 11:30 AM	Break	
11:30 AM to 1:00 PM	Gour P Das	Implementations of DFT via basis sets
1:00 PM to 2:00 PM	Lunch	
2:00 PM to 3:00 PM	Phani Motamari	Large-scale DFT calculations using finite element basis in exa-scale era
3:00 PM to 4:30 PM	Biplab Sanyal and Subhradip Ghosh	Interpretation of DFT results
4:30 PM to 5:00 PM	Break	
5:00 PM to 6:30 PM	Poster Session	
23- July		
9:30 AM to 11:00 AM	Tanmoy Das	Role of symmetry and topology in condensed matter physics
11:00 AM to 11:30 AM	Break	
11:30 AM to 1:00 PM	Indra Dasgupta	Model Hamiltonians
1:00 PM to 2:00 PM	Lunch	
2:00 PM to 3:00 PM	K.B.Maiti	Experimental validation of DFT
3:00 PM to 4:30 PM	Manoj Harbola	Recent advances in DFT

4:30 PM to 5:00 PM	Break	
5:00 PM to 6:30 PM	Poster Session	
6:30 PM to 7:30 PM	Special Lecture by Bhupendra Dev	The rise of quantum computing: challenges and opportunities
24- July		
9:30 AM to 10:30 AM	Abhishek Sharma	Quantum Transport
10:30 AM to 11:30 AM	Srinivasa Prasanna V	Quantum algorithms (Online)
11:30 AM to 12:00 Noon	Break	
12:00 Noon to 1:00 PM	Arti Kashyap	DFT and Machine learning
1:00 PM to 2:00 PM	Lunch	

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Conference Schedule

24- July (Conference)		
Session: Machine learning for materials science Chair: Manoj Harbola		
2:00 PM to 2:30 PM	Hemanadhan Myneni	Machine Learning-Assisted Quantum Simulations for Photoactive Materials
2:30 PM to 3:00 PM	Biswarup Pathak	Development of Artificially Intelligent Nanopores for High-Throughput DNA Sequencing
3:00 PM to 3:30 PM	Break	
3:30 PM to 4:00 PM	Tanmoy Paul	Novel Na-ion Battery Cathodes Prediction using Machine Learning and Density Functional Theory Approach
4:00 PM to 4:30 PM	Saurabh Ghosh	Hypothesis-driven active learning and causal relations for functional materials
4:30 PM to 5:00 PM	Break	
Session: Experimentalist perspective Chair: Biplab Sanyal		
5:00 PM to 5:30 PM	Venkata Kamalakar	TBA [ONLINE]
5:30 PM to 6:30 PM	Break	
6:30 PM to 7:30 PM	Special Talk: PK Ahluwalia Transformative Interventions in Physics Education: IAPT'S Journey of Four Decades Chair: Arti Kashyap	
25- July		
Session: Topology in quantum materials Chair: P.K.Ahluwalia		
09:00 AM to 09:30 AM	Bahadur Singh	Atomically thin obstructed atomic insulators in puckered lattice materials
09:30 AM to 10:00 AM	Awadhesh Narayan	Non-Linear Hall Effect in Flatlands and Chiral Crystals
10:00 AM to 10:30 AM	Poorva Singh	Exploring Novel Topological Phases in 3D Materials: Theoretical Insights and Predictions

10:30 AM to 11:00 AM	Mukhtiyar Singh	Emergence of topological phase and non-trivial surface states in rare-earth mono pnictide semimetals
11:00 AM to 11:30 AM	Break	
Session: Exotic quantum effects Chair: B.N.Dev		
11:30 AM to 12:00 Noon	Arghya Taraphder	NbSe ₂ /MoS ₂ heterostructure: A candidate for Ising superconductivity
12:00 Noon to 12:30 PM	Anil Prabhakar	Chemistry in the Era of Quantum Computers
12:30 PM to 1:00 PM	Kartick Tarafder	Unravelling the intriguing phenomena in low dimensional bio-metal-organic frameworks and their interfaces
1:00 PM to 2:00 PM	Lunch	
2:00 PM to 2:30 PM	Conference Photo	
2:30 PM to 4:00 PM	Celebration of Prof GP Das's 70th Birthday	
4:00 PM to 5:30 PM	Departure to Mandi	Local sightseeing/ Meetings with speakers/ Rest/ Or anything else
7:00 PM	Conference Dinner at Rajmahal, Mandi Town	
10:00 PM	Back to Campus	
26- July		
Session: Magnetism in 2D materials Chair: Arghya Tarafder		
9:30 AM to 10:00 AM	Mukul Kabir	Unleashing two-dimensional magnetism in ultrathin oxide flakes
10:00 AM to 10:30 AM	Nirmal Ganguli	Understanding broken-symmetry antiferromagnets through group theory and DFT calculations
10:30 AM to 11:00 AM	Swarup Kumar Panda	Frustrated Magnetism and electronic structure of CaMn ₂ P ₂
11:00 AM to 11:30 AM	Break	
Session: Spin-orbit related phenomena Chair: Indra Dasgupta		
11:30 PM to 12:00 Noon	Amrita Bhattacharya	Exploring the spin-orbit driven Rashba splitting in Perovskite oxides
12:00 Noon to 12:30 PM	Sudip Chakraborty	Computational Roadmap of Emerging Materials: Implications of Piezochromism and Rashba Physics
12:30 PM to 1:00 PM	Gargee Sharma	Localization beyond Dirac and Weyl fermions

1:00 PM to 2:00 PM	Lunch	
Session: Energy materials Chair: G. P. Das		
2:00 PM to 2:30 PM	Chiranjib Majumder	Modelling of Energy Materials using DFT Approach: Implications for H-Economy
2:30 PM to 3:00 PM	Koushik Pal	Electron-Phonon Interaction Mediated Giant Enhancement of Electron Transport Properties Induced by Topological Phase Transition
3:00 PM to 3:30 PM	Break	
3:30 PM to 4:00 PM	Tisita Das	Computational Advancement for Next-Generation Energy Materials and Neuromorphic Paradigm
4:00 PM to 4:30 PM	Shivam Tripathi	How Poisoning Is Avoided in a Step of Relevance to the Haber–Bosch Catalysis
4:30 PM to 5:00 PM	Closing Ceremony	