

ESTESODP – 2024 School Schedule (11<sup>th</sup> -12<sup>th</sup> Nov 2024)

Time	Session	Speaker
11-Nov-2024 (Monday) Chairperson: Prof. G. P. Das Venue: SJSOM		
08:00 AM - 09:00 AM	Registration	
09:00 AM - 10:15 AM	Fundamentals and application of density functional theory	Prof. Biplab Sanyal
10:15 AM - 11:30 AM	Density functional theory across different length scales: Quantum and classical	Prof. Swapan Ghosh
11:30 AM - 12:00 PM	Tea Break	
12:00 PM - 01:15 PM	An introduction to spin-orbit driven emergent phases	Prof. Indra Dasgupta
01:15 PM - 02:30 PM	Lunch Break	
Tutorials Venue: Bits and Bytes Lab		
02:30 PM - 04:00 PM	Tutorial 1: Basics of DFT calculations - self consistent loops and geometry optimization	
04:00 PM - 04:30 PM	Tea Break	
04:30 PM - 06:00 PM	Tutorial 2: Electronic structure using DFT - band structures and density of states	
Dinner		
12-Nov-2024 (Tuesday) Chairperson: Prof. Biplab Sanyal Venue: SJSOM		
09:00 AM - 10:15 AM	Introduction to classical and Ab initio molecular dynamics simulation	Prof. Dilip Kanhere
10:15 AM - 11:30 AM	Berry phase in quantum physics of solids with some case studies	Prof. Gour Prasad Das
11:30 AM - 12:00 PM	Tea Break	
12:00 PM - 01:15 PM	Exploring electronic structure through spectroscopy	Prof. Kalobaran Maiti
01:15 PM - 02:30 PM	Lunch Break	
Tutorials Venue: Bits and Bytes Lab		
02:30 PM - 04:00 PM	Tutorial 3: Magnetism using DFT - magnetic ground states and anisotropy	
04:00 PM - 04:30 PM	Tea Break	
04:30 PM - 06:00 PM	Tutorial 4: Calculation of isotropic magnetic exchange by energy mapping method	
Dinner		

# ESTESODP – 2024 Conference Schedule (13<sup>th</sup> -15<sup>th</sup> November 2024)

Day 1, 13/11/2024 (Wednesday)	
09:00 AM – 09:30 AM	Registration
09:30 AM – 10:00 AM	Welcome Address by Organizers, DD-ART, Dean R&D, HoD MEMS
<b>Session Chair: Alok Shukla (IIT, Bombay)</b> <b>Venue: P C Saxena</b>	
10:00 AM – 10:45 AM	<b>Shobhana Narasimhan (JNCASR, Bangalore)</b> <b>Title:</b> At Cross Purposes: Spin-crossover systems on metal substrates
10:45 AM – 11:30 AM	<b>Swapn K. Pati (JNCASR, Bangalore)</b> <b>Title:</b> Computational modelling of transport phenomena in a few semiconductors
<b>11:30 AM – 12:00 PM</b> <b>Tea Break</b>	
<b>Session Chair: K. G. Suresh (IIT, Bombay)</b> <b>Venue: P C Saxena</b>	
12:00 PM – 12:30 PM	<b>Abir De Sarkar (INST, Mohali)</b> <b>Title:</b> DFT perspectives on spin-orbitronics and piezotronics in selected functional 2D materials
12:30 AM – 01:00 PM	<b>Prasenjit Ghosh (IISER, Pune)</b> <b>Title:</b> Theoretical prediction of ZrHfCoNiSnSb high entropy half Heusler alloy with low lattice thermal conductivity
<b>01:00 PM – 02:00 PM</b> <b>Lunch Break</b>	
<b>Session Chair: Ashok Arya (BARC, Mumbai)</b> <b>Venue: SJSOM</b>	
02:00 PM – 02:30 PM	<b>Debjani Karmakar (BARC, Mumbai)</b> <b>Title:</b> Intriguing role of spin-orbit coupling on magnetic chirality of systems with broken inversion symmetries: Two examples
02:30 PM – 03:00 PM	<b>Mukul Kabir (IISER, Pune)</b> <b>Title:</b> Hole-doped two-dimensional magnets
03:00 PM – 03:30 PM	<b>Sayantika Bhowal (IIT, Bombay)</b> <b>Title:</b> Spin-orbit coupling in ferroaxial materials: Driving the fourth ferroic order and hidden spin polarization
<b>03:30 PM – 04:00 PM</b> <b>Tea Break</b>	
<b>Session Chair: Swapn Pati (JNCASR, Bangalore)</b> <b>Venue: SJSOM</b>	
04:00 PM – 04:30 PM	<b>Ashok Arya (BARC, Mumbai)</b> <b>Title:</b> Probing magnetic and defect structures in oxides/mixed oxides
04:30 PM – 05:00 PM	<b>Subhradip Ghosh (IIT, Guwahati)</b> <b>Title:</b> Non-volatile electrically switchable half-metallicity in multiferroic TMDC-MXene heterostructures

05:00 PM – 05:30 PM	<b>Dipanshu Bansal (IIT, Bombay)</b> <b>Title:</b> Strong orbital-selective spin-orbital-phonon coupling in CrVO <sub>4</sub>
Contributed oral 05:30 PM to 06:30 PM	<b>Soheil Ershadrad (Uppsala University, Sweden)</b> <b>Title:</b> Ab initio study of magnetic properties in 2D metallic magnets: A case study of the Fe <sub>n</sub> GeTe <sub>2</sub> family and FeNbTe <sub>2</sub>
	<b>Ted Trewick (Victoria University of Wellington, New Zealand)</b> <b>Title:</b> Anisotropic magnetoresistance in Gadolinium Nitride
	<b>Krishnaraj K (IIT, Bombay)</b> <b>Title:</b> Unraveling the Rashba-Dresselhaus effect and spin switching in ferroelectric AlO <sub>3</sub> (A=K, Rb, Cs, Tl) perovskites
	<b>Bishal Das (IIT, Bombay)</b> <b>Title:</b> Coexistence of altermagnetism and Topological Weyl fermions in GdAlSi
07:30 PM – 09:30 PM Dinner at Padma Vihar	

Day 2, 14/11/2024 (Thursday)	
Session Chair: Shobhana Narasimhan (JNCASR, Bangalore)	
Venue: SJSOM	
09:00 AM – 09:45 AM	<b>Lars Nordström (Uppsala University, Sweden)</b> <b>Title:</b> Spin-orbit coupling and its dependence on magnetic symmetry applied to the enigmatic case Mn <sub>3</sub> Sn
09:45 AM – 10:30 AM	<b>Priya Mahadevan (SNBNCBS, Kolkata)</b> <b>Title:</b> Examining the ground state of the Slater insulator NaOsO <sub>3</sub>
10:30 AM – 11:00 AM Tea Break	
Session Chair: Hridis Kumar Pal (IIT, Bombay)	
Venue: SJSOM	
11:00 AM – 11:30 AM	<b>Bahadur Singh (TIFR, Mumbai)</b> <b>Title:</b> Spin U(1) quasi-symmetry in materials with a quantized spin Hall effect
11:30 AM – 12:00 PM	<b>Awadhesh Narayan (IISc, Bangalore)</b> <b>Title:</b> Non-linear hall effect in flatlands and chiral crystals
12:00 PM – 12:30 PM	<b>Swarup Panda (Bennett University, Delhi)</b> <b>Title:</b> Spin-spiral magnetism in Honeycomb lattice of CaMn <sub>2</sub> P <sub>2</sub> - A first-principles and monte carlo perspective
Contributed oral 12:30 PM – 01:00 PM	<b>Rajnarayan De (BARC, Andhra Pradesh)</b> <b>Title:</b> Electronic and thermoelectric properties of 1-quintuple layer chalcogenides
	<b>Kausar Ali (BARC, Mumbai)</b> <b>Title:</b> First-principles study of Titanite-Type CaTiSiO <sub>5</sub> under pressure
01:00 PM – 02:00 PM Lunch Break	
Session Chair: Avradeep Pal (IIT, Bombay)	
Venue: SJSOM	
02:00 PM – 02:30 PM	<b>Shouvik Chatterjee (TIFR, Mumbai)</b> <b>Title:</b> Controlling Hall response in epitaxial Mn <sub>3</sub> Sn thin films
02:30 PM – 03:00 PM	<b>Jackson Miller (Victoria University of Wellington, New Zealand)</b> <b>Title:</b> Experiment, computation, and a possible quantum critical point in SmN

03:00 PM – 03:30 PM	<b>Titas Dasgupta (IIT, Bombay)</b> <b>Title:</b> A refinement-based approach for extracting electronic band structure information and its application in thermoelectric materials and devices
03:30 PM – 05:45 PM	<b>Tea Break</b> <b>&amp;</b> <b>Poster presentations by student participants</b>
<b>06:00 PM – 10:30 PM</b> <b>Banquet Dinner</b>	

<b>Day 3, 15/11/2024 (Friday)</b>	
<b>Session Chair: Gopalan Rajaraman (IIT, Bombay)</b> <b>Venue: SJSOM</b>	
09:30 AM – 10:00 AM	<b>Ankit Jain (IIT, Bombay)</b> <b>Title:</b> Phonon thermal transport in low- and high-thermal conductivity solids
10:00 AM – 10:30 AM	<b>Chiranjib Majumdar (BARC, Mumbai)</b> <b>Title:</b> Nano-ring to Nano-barrel: structural evolution of CuO clusters
10:30 AM – 11:00 AM	<b>Ranjit Thapa (SRM University, Amravati)</b> <b>Title:</b> Beyond d-band center to identify the catalyst for oxygen evolution reaction
<b>11:00 AM – 11:30 AM</b> <b>Tea Break</b>	
<b>Session Chair: Priya Mahadevan (S. N. Bose, Kolkata)</b> <b>Venue: SJSOM</b>	
11:30 AM – 12:00 PM	<b>Saurabh Ghosh (SRM University, Chennai)</b> <b>Title:</b> Polarization coupled magnetization switching in oxide perovskites
12:00 PM – 12:30 PM	<b>Partha Sarathi Ghosh (BARC, Mumbai)</b> <b>Title:</b> Coupling of the structure and magnetism to spin splitting in hybrid organic-inorganic perovskites
12:30 PM – 01:00 PM	<b>B. R. K. Nanda (IIT, Chennai)</b> <b>Title:</b> Realizing Friedel oscillation in the orbital channel: valley driven physics of NbSe <sub>2</sub> with a magnetic impurity
<b>01:00 PM – 02:00 PM</b> <b>Lunch Break</b>	
<b>Session Chair: Saumya Bera (IIT, Bombay)</b> <b>Venue: SJSOM</b>	
02:00 PM – 02:30 PM	<b>Rudra Banerjee (SRM University, Chennai)</b> <b>Title:</b> Data-driven discovery of quantum compatible deep centers in semiconductors
02:30 PM – 03:00 PM	<b>Sudipta Kanungo (IIT, Goa)</b> <b>Title:</b> Strategic role played by the SOC in emerging magnetic and topological phases in oxides and alloys
03:00 PM – 03:30 PM	<b>Arnab Bose (IIT, Kanpur)</b> <b>Title:</b> Generation of efficient spin currents in topological and altermagnetic materials
<b>03:30 PM – 04:00 PM</b> <b>Tea Break</b>	

<b>Session Chair: Saurabh Ghosh (SRM University, Chennai)</b> <b>Venue: SJSOM</b>	
Contributed oral 04:00 PM – 05:15 PM	<b>Shovan Gayen (Bennett University, Delhi)</b> <b>Title:</b> Pressure induced electronic and magnetic transition in antiferromagnetic NiS: A combined DFT+U and Monte-Carlo study
	<b>Dipanwita Bhattacharjee (IIT, Bombay)</b> <b>Title:</b> Effect of spin-orbit coupling on the thermoelectric power factor of CoBi based half-Heusler compounds
	<b>Jagjit Kaur (HRI, Allahabad)</b> <b>Title:</b> Unraveling Rashba effect through spin-texture evolution in unidimensional-confined halide-perovskite under compression
	<b>P. Gayathri (SRM University, Chennai)</b> <b>Title:</b> Machine learning and atomistic simulations for predicting ferroelectric switching in hybrid improper ferroelectric double perovskites oxides
	<b>Joydeep Majhi (IIT, Bombay)</b> <b>Title:</b> Investigating magneto-caloric effect and exchange interaction in NdMnO <sub>3</sub> perovskite: A computational study
05:15 PM - 05:45 PM	<b>Presentation by sponsors</b>
06:00 PM – 06:30 PM	<b>Award Ceremony and words from organizers</b>
06:30 PM – 07:00 PM	<b>Concluding Remarks by panel members</b>
<b>07:30 PM – 09:30 PM</b> <b>Dinner at Padma Vihar</b>	