International Workshop and Conference on

Evolution of Electronic Structure Theory and Experimental Realization (EESTER 2020)

Jointly Organized by SRM IST KTR (India), IIT Madras (India) and Uppsala University (Sweden)

December 14- 18, 2020 in online mode

Inaugural Session: Day 1, 14th December 2020, Monday

8:30 am - 9:00 am (Central European Time) / 1:00 pm - 1:30 pm (Indian Standard Time)

Program Schedule	Day 1 14th December Monday	Day 2 15th December Tuesday	Day 3 16th December Wednesday	Day 4 17th December Thursday	Day 5 18th. December Friday

PL = Plenary Lecture
(45 minutes talk + 15 minutes discussion)
WL = Workshop Lecture
(45 minutes talk + 15 minutes discussion)
SL = Seminar Lectures
(30 minutes talk + 10 minutes discussion)
CET = Central European Time

OP = Oral Presentations
(12 minutes talk + 3 minutes discussion)
PO= POSTER Presentations
(3 minutes pre-recorded YouTube Video link
+ 2 minutes Q&A)

IST = Indian Standard Time

Demonstration of Electronic Structure code Quantum Espresso

- Day 4: 10:00 am – 12:30 pm (IST) for participants login from India
- Day 4: 3:00 pm - 5:30 pm (CET) for participants login from Europe/US/Brazil

Day 1: 14th December, Session 1, 9:00 am – 12:00 pm CET / 1:30 pm – 4:30 pm IST

PL1: Theory

CET 9:00 am – 10:00 am
IST 1:30 pm – 2:30 pm

Prof. G. Baskaran, IIT Madras, India, IMSc, Chennai, India & Perimeter Institute, Waterloo, Canada

Theory of Electronic Structures from Experimental Results - The Anderson Way

PL2: Theory

CET 10:00 am – 11:00 am
IST 2:30 pm – 3:30 pm

Prof. Olle Eriksson, Uppsala University, Sweden

DFT and fundamentals of electronic structure calculations

PL3: Experiment

CET 11:00 am – 12:00 pm
IST 3:30 pm – 4:30 pm

Prof. D. D. Sarma, Indian Institute of Science Bangalore, Bengaluru, India

An introduction to photoelectron spectroscopy: How to estimate electronic parameter strengths from experiments

Break 20 Minutes : 12:00 pm – 12:20 pm (CET) / 4:30 pm - 4:50 pm (IST)

Day 1: 14th December, Session 2, 12:20 pm – 3:30 pm CET / 4:50 pm – 8:00 pm IST

POSTER (PO)

CET 12:20 pm -12:40 pm
IST 4:50 pm – 5:10 pm

POSTER Theory Application (PTA)-1, 2, 3, 4

SL1: Theory CET 12:40 pm – 1:20 pm IST 5:10 pm – 5:50 pm	 **Prof. Hena Das,** Tokyo Institute of Technology, Yokohama, Japan *Microscopic origin of near room-temperature multiferroic phenomena in $(LuFeO_3)_m/(LuFe_2O_4)_1$ superlattices*
SL2: Experiment CET 1:20 pm -2:00 pm IST 5:50 pm -6:30 pm	 **Prof. A. Sundaresan,** JNCASR, Bangalore, India *Multiferroic Properties and Unconventional Spin Density Wave in Doubly Ordered Perovskite $NaLnNiWO_6$ (Ln=Y, Dy, Ho, and Yb)*
SL3: Theory CET 2:00 pm – 2:40 pm IST 6:30 pm - 7:10 pm	 **Prof. Biswarup Pathak,** Indian Institute of Technology Indore, India *Nano-electrodes for ultrafast DNA sequencing*
POSTER (PO) CET 2:40 pm - 3:00 pm IST 7:10 pm – 7:30 pm	**POSTER Theory Application (PTA)- 5,6,7,8**
POSTER (PO) CET 3:00 pm – 3.30 pm IST 7:30 pm - 8:00 pm	**Open Forum Discussion on POSTER presentations**

Day 2: 15th December, Session 1, 9:00 am – 12:00 pm CET / 1:30 pm – 4:30 pm IST	
WL1: Theory CET 9:00 am – 10:00 am IST 1:30 pm – 2:30 pm	 **Prof. G.P. Das,** Indian Institute of Technology Kharagpur, India *DFT in condensed systems : some practical guidelines*
WL2: Theory CET 10:00 am – 11:00 am IST 2:30 pm – 3:30 pm	 **Prof. Aftab Alam,** Indian Institute of Technology Bombay, Mumbai, India *Broken symmetry driven topological semi-metal to gaped phase transition in SrAgAs*
WL3: Theory CET 11:00 am – 12:00 pm IST 3:30 pm – 4:30 pm	 **Prof. Indra Dasgupta,** Indian Association for the Cultivation of Science, Kolkata, India *Modeling Strongly Correlated Systems*
Break 20 Minutes : 12:00 pm – 12:20 pm (CET) / 4:30 pm - 4:50 pm (IST)	
Day 2: 15th December, Session 2, 12:20 pm – 3:30 pm CET / 4:50 pm – 8:00 pm IST	

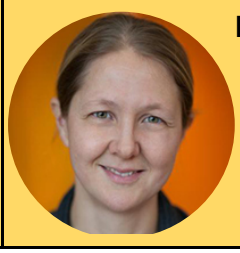
POSTER (PO) CET 12:20 pm -12:40 pm IST 4:50 pm – 5:10 pm	**POSTER Theory Application (PTA)- 9,10,11,12**
SL4: Theory CET 12:40 pm – 1:20 pm IST 5:10 pm – 5:50 pm	 **Prof. Alessandro Stroppa,** CNR-SPIN, Italy *Electric dipole ordering and spin-orbit interaction in hybrid organic-inorganic perovskites*
SL5: Theory CET 1:20 pm -2:00 pm IST 5:50 pm -6:30 pm	 **Prof. Tanmoy Das,** Indian Institute of Science Bangalore, India *Topological phases of matter*
PL4: Theory CET 2:00 pm -3.00 pm IST 6:30 pm - 7:30 pm	 **Prof. Sokrates Pantelides** Vanderbilt University, Nashville, USA *Adventures and discoveries in layered two-dimensional ferroelectrics*
POSTER (PO) CET 3:00 pm – 3.30 pm IST 7:30 pm - 8:00 pm	**POSTER Theory Application (PTA)- 13,14,15,16,17, 18**

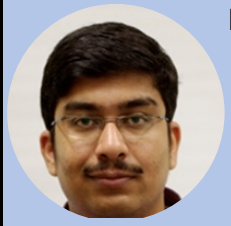
Day 3: 16th December, Session 1, 9:00 am – 12:00 pm CET / 1:30 pm – 4:30 pm IST

PL5: Machine Learning CET 9:00 am – 10:00 am IST 1:30 pm – 2:30 pm	 **Prof. Tamio Oguchi,** Osaka University, Japan *Machine Learning Applied to Materials Science*
Oral Presentations (OP) CET 10:00 am – 11:00 am IST 2:30 pm – 3:30 pm **OTD= ORAL Theory Development**	**OTD-1: Bikash Patra**, National Institute of Science Education and Research, Bhubaneswar, India *Relevance of the Pauli kinetic energy density for semilocal functional* **OTD-2: Dr. Igor Di Marco,** Asia Pacific Center for Theoretical Physics, South Korea *Determining the Intra-Atomic Exchange Energy in Rare-Earth Adatoms* **OTD-3: Aditi Mandal,** Birla Institute of Technology and Science, Pilani, India *Brief description of Plasmon excitation within multiple scattering approach Photoemission energy loss spectroscopy* **OTD-4: Dr. Subhayan Roychoudhury**, Lawrence Berkeley National Laboratory, USA *Neutral excitation density functional theory: a variational first-principles method for simulating excitations in molecules*

Oral Presentations (OP) CET 11:00 am – 12:00 pm IST 3:30 pm – 4:30 pm **OTA= ORAL Theory Application**	**OTA-1: Santanu Pathak**, Variable Energy Cyclotron Centre, Kolkata, India *Precision measurement and electronic structure calculations for understanding the microscopic and macroscopic properties of HfO_2* **OTA-2: Namrata Jaykhedkar,** Faculty of Natural Sciences, Slovakia *Theoretical study of temperature dependent behaviour of crystal phase in $SrZrS_3$* **OTA-3: Shashi Bhusan Mishra,** IIT Madras, Chennai, India *Formation of a suspended magnetic layer between graphene layers through fluorine intercalation* **OTA-4: Dr. Tisita Das,** Harish-Chandra Research Institute, Allahabad, India *Enhanced Hydrogen Evolution Activity at the Edges of $MPSe_3$ (M=Mn, Fe) Tri-chalcogenide Layers*
Break 20 Minutes : 12:00 pm – 12:20 pm (CET) / 4:30 pm - 4:50 pm (IST)	
Day 3: 16th December, Session 2, 12:20 pm – 3:30 pm CET / 4:50 pm – 8:00 pm IST	
POSTER (PO) CET 12:20 pm -12:40 pm IST 4:50 pm – 5:10 pm	**POSTER Theory Development (PTD)-1,2** **POSTER Theory Application (PTA)- 19, 20**
SL6: Machine Learning CET 12:40 pm – 1:20 pm IST 5:10 pm – 5:50 pm	 **Prof. Ranjit Thapa** SRM University-AP, Amravati, India *Descriptor to define the activity of carbon catalyst for OER: Quantum Mechanics and Machine Learning Approach*
SL7: Machine Learning CET 1:20 pm -2:00 pm IST 5:50 pm -6:30 pm	 **Prof. Tarak Patra** Indian Institute of Technology Madras, Chennai, India *Deep Learning and Active Learning of Interatomic Force Fields*
PL6: Machine Learning CET 2:00 pm – 3.00 pm IST 6:30 pm - 7:30 pm	 **Prof. Rampi Ramprasad,** Georgia Tech, USA *Polymer Informatics: Current Status & Critical Next Steps*
POSTER (PO) CET 3:00 pm – 3.30 pm IST 7:30 pm - 8:00 pm	**POSTER Theory Application (PTA)- 21, 22, 23, 24, 25**
Day 4: 17th December, Session 1, 9:00 am – 12:00 pm CET / 1:30 pm – 4:30 pm IST	
PL7: Experiment CET 9:00 am – 10:00 am IST 1:30 pm – 2:30 pm	 **Prof. Joachim Mayer,** RWTH Aachen University, Germany *Atomic Scale Imaging and Spectroscopy with Aberration Corrected Transmission Electron Microscopy*

WL4: Experiment CET 10:00 am – 11:00 am IST 2:30 pm – 3:30 pm	 **Prof. Kalobaran Maity,** Tata Institute of Fundamental Research, Mumbai, India *Spectroscopy for electronic structure analysis*
WL5: Experiment CET 11:00 am – 12:00 pm IST 3:30 pm – 4:30 pm	 **Prof. Bent Weber,** Nanyang Technological University, Singapore *Proximity-Induced Superconductivity in Epitaxial Quantum Spin Hall Heterostructures*
Break 20 Minutes : 12:00 pm – 12:20 pm (CET) / 4:30 pm - 4:50 pm (IST)	
Day 4: 17th December, Session 2, 12:20 pm – 3:30 pm CET / 4:50 pm – 8:00 pm IST	
CET 12:20 pm -12:40 pm IST 4:50 pm – 5:10 pm	**Open Forum for Discussion on Demonstration of Quantum Expresso**
SL8: Experiment CET 12:40 pm – 1:20 pm IST 5:10 pm – 5:50 pm	 **Prof. Srimanta Middey,** Indian Institute of Science, Bangalore, India *Defect induced emergent phenomena at the surface and interface of band insulators*
SL9: Experiment CET 1:20 pm -2:00 pm IST 5:50 pm -6:30 pm	 **Prof. Ravi Singh,** IISER Bhopal, India *Role of Disorder, Spin Orbit Coupling and Magnetism in the Electronic Structure of Ir Based Double Perovskite*
PL8: Theory CET 2:00 pm – 3.00 pm IST 6:30 pm - 7:30 pm	 **Prof. Lars Nordstrom,** Uppsala University, Sweden Complex magnetic order and their spontaneous spin and charge currents
CET 3:00 pm – 3.30 pm IST 7:30 pm - 8:00 pm	Demonstration: Quantum Espresso for participants login from outside India contd.

Day 5: 18th December, Session 1, 9:00 am – 12:00 pm CET / 1:30 pm – 4:30 pm IST	
PL9: Theory CET 9:00 am – 10:00 am IST 1:30 pm – 2:30 pm	 **Prof. Annica Black-Schaffer,** Uppsala University, Sweden *Topological superconductivity and Majorana fermions*

WL6: Machine Learning CET 10:00 am – 11:00 am IST 2:30 pm – 3:30 pm	 **Prof. Abhishek Singh,** Indian Institute of Science Bangalore, India *Machine learning and its application in Materials Science: Role of various Algorithms*
WL7: Experiment CET 11:00 am – 12:00 pm IST 3:30 pm – 4:30 pm	 **Prof. Avinash V. Mahajan,** Indian Institute of Technology Bombay, India *Novel states in magnetism: low-dimensional systems and spin liquids*
Break 20 Minutes : 12:00 pm – 12:20 pm (CET) / 4:30 pm. - 4:50 pm (IST)	
Day 5: 18th December, Session 2, 12:20 pm – 3:20 pm CET / 4:50 pm – 7:50 pm IST	
ORAL Presentations CET 12:20 pm – 1:20 pm IST 4:50 pm – 5:50 pm Oral Presentations Experiment (OEX)	**OEX-1: Abhishek Maiti**, Indian Association for the cultivation of Science, Kolkata, India *Rashba Band Splitting in Methylammonium Lead Iodide: An Insight from Spin-Polarized Scanning Tunnelling Spectroscopy* **OEX-2: Sameer Kumar Mallik,** Institute of Physics, Bhubaneswar, India *Hysteresis study in salt-assisted CVD grown monolayer MoS2 field-effect transistor by pulsed I~V technique* **OEX-3: Dr. Rajib Batabyal,** Niels Bohr Institute, Denmark *Topological Fermi-arcs and Weyl node connectivity in ferromagnetic Weyl semimetal $Co_3Sn_2S_2$* **OEX-4: Dr. Sofi Suhail Majid,** Institute of Physics, Taiwan *Unveiling the role of V-V dimerization on insulator-metal transition and optical transmittance of VO_2 thin films*
Oral Presentations CET 1:20 pm – 1:45 pm IST 5:50 pm – 6:15 pm	**POSTER Experiment (OEX)-1,2,3,4,5**
CET 1:45 pm – 2:05 pm IST 6:15 pm – 6:35 pm	**Open slot for discussion / reschedule talk**
SL10: Experiment CET 2:00 pm – 2.40 pm IST 6:35 pm - 7:15 pm	 **Prof Shibayan Roy** Indian Institute of Technology Kharagpur, Kharagpur, India *Atomic scale experimental characterization complimented by atomic scale simulations for component scale materials designing*
Concluding Session CET 2:45 pm – 3.15 pm IST 7:15 pm – 7:45 pm	**Prize Distribution, Feedback from Participants & Vote of Thanks** Biplab Sanyal, Ranjit Nanda, Sudakar Chandran, Saurabh Ghosh, Jaivardhan Sinha and other invited guests