

EESTER 2020 – POSTER Presentations

SL. No	Name & Affiliation	Title	Category	Presentation Number	Schedule
1	Sujoy Datta Department of Physics, University of Calcutta, West Bengal, India	Semi-local DFT Advancement on Full Potential Localized Basis Scheme for Semiconductor Band-gap Prediction and Beyond	Theory Development - POSTER 1	PTD-1	Day 3 16 th Dec. 4:50 pm IST (5 minutes)
2	Dr. Nisha Singh, Technical University Delft, Netherlands	Manipulation of magnon modes in alloys	Theory Development - POSTER 2	PTD-2	Day 3 16 th Dec. 4:55 pm IST (5 minutes)
3	Dr. Sri Kasi Matta, RMIT University, Australia	Two-dimensional (2D) Transition metal chalcogenides (TcX ₂ , X=S, Se) for charge transport in Perovskite Solar Cells: A DFT study	Theory Application - POSTER 1	PTA-1	Day 1 14 th Dec. 4:50 pm IST (5 minutes)
4	Joydipto Bhattacharya, Raja Ramanna Centre for Advanced Technology, Indore, India	Unusual magnetic and electronic properties of Al-substituted Ga ₂ MnNi: An ab initio study	Theory Application - POSTER 2	PTA-2	Day 1 14 th Dec. 4:55 pm IST (5 minutes)
5	Dr. Badiur Rahaman, Aliah University, Department of Physics, IIA/27-Newtown, Kolkata, India	Electronic properties and microscopic modeling of Polymeric Fe(II) triazole	Theory Application - POSTER 3	PTA-3	Day 1 14 th Dec. 5:00 pm IST (5 minutes)
6	Saumen Chaudhuri, IIT Kharagpur, West Bengal, India	Functionalization of monolayer MoS ₂ by applying mechanical strain	Theory Application - POSTER 4	PTA-4	Day 1 14 th Dec. 5:05 pm IST (5 minutes)
7	Rajeev Dutt, Raja Ramanna Centre of Advanced Technology, Indore, India	Probing the martensitic transition and thermoelectric properties of Co _x TaZ (Z=Si,Ge,Sn and x=1,2) : a study based on DFT	Theory Application - POSTER 5	PTA-5	Day 1 14 th Dec. 7:10 pm IST (5 minutes)
8	Aditya Shrvan Shende, Visvesvaraya National Institute of Technology (VNIT), S Ambazari Rd, Ambazari, Nagpur, Maharashtra, 440010, India	Exploration of Electronic and Topological Properties of Strain Induced Transition metal trichalcogenides Materials	Theory Application - POSTER 6	PTA-6	Day 1 14 th Dec. 7:15 pm IST (5 minutes)
9	Akshay Mahajan Indian Institute of Technology Kanpur, Punjabi Mohalla Baharli Bundi, Bundi (Rajasthan) 323001, India	Strain-engineering-based study of 2D Multiferroic VOCl ₂ Monolayer	Theory Application - POSTER 7	PTA-7	Day 1 14 th Dec. 7:20 pm IST (5 minutes)

10	Mandira Das, Department of Physics, IIT Guwahati, Amingaon North Guwahati, Assam, India	Calculation of Quantum Capacitance and Pseudo- capacitance of Ti, Nb, Mo, V based Pristine and O- functionalized MXene using Density	Theory Application - POSTER 8	PTA-8	Day 1 14 th Dec. 7:25 pm IST (5 minutes)
11	Samarendra Roy, Indian Institute of Technology, Kharagpur West Bengal 721302 Country: India	Effect of Mn on the precipitation kinetics of Al-Cu alloy	Theory Application - POSTER 9	PTA-9	Day 2 15 th Dec. 4:50 pm IST (5 minutes)
12	Mahendiran Durairaj, CSIR-Central Electro Chemical Research Institute, Chennai, India	Understanding the Stability of Edge States in SiC Nanoribbons by First Principles Approach	Theory Application - POSTER 10	PTA-10	Day 2 15 th Dec. 4:55 pm IST (5 minutes)
13	Halima Said, Department of Physical and Theoretical Chemistry and Laboratory of Advanced Materials, Faculty of Natural Sciences, Comenius University, Ilkovicova 6, SK- 84215 Bratislava, Slovakia	Ab-initio molecular dynamics study of cesiated molybdenum surfaces	Theory Application - POSTER 11	PTA-11	Day 2 15 th Dec. 5:00 pm IST (5 minutes)
14	Dr. Debolina Misra Department of Metallurgical and Materials Engineering, IIT Madras, Chennai, India	Transition metal implanted oxide as support for noble metal single atoms	Theory Application - POSTER 12	PTA-12	Day 2 15 th Dec. 5:05 pm IST (5 minutes)
15	Rayan Chakraborty, Indian Institute of Science Education and Research (IISER), Pune, India	Thermodynamics of Hydrogen Evolution from Surfaces of Earth-abundant Cu ₂ BaSnS ₄	Theory Application - POSTER 13	PTA-13	Day 2 15 th Dec. 7:30 pm IST (5 minutes)
16	Marcelo Albuquerque, Universidade Federal Fluminense (UFF), Brazil	XANES simulations in diamond- like two-dimensional material	Theory Application - POSTER 14	PTA-14	Day 2 15 th Dec. 7:35 pm IST (5 minutes)
17	Deepak S. Gavali, SRM University – AP, Andra Pradesh, India	Synergetic effect of localized and delocalized π electron on Li storage properties of Si/C heterostructures	Theory Application - POSTER 15	PTA-15	Day 2 15 th Dec. 7:40 pm IST (5 minutes)
18	Khorsed Alam Harish-Chandra Research Institute. Chhatnag Road, Jhunsi, Prayagraj (Allahabad), Uttar Pradesh, India	DFT study into efficient bifunctional catalytic activity of cobalt dispersed N-doped graphitic nanospheres in Zn-air battery	Theory Application - POSTER 16	PTA-16	Day 2 15 th Dec. 7:45 pm IST (5 minutes)

19	Aswathi Mohan T Institute of Science Education and Research (IISER), Pune, India	CO ₂ capture, activation and dissociation on the Ti ₂ C surface and Ti ₂ C MXene: the role of surface structure	Theory Application - POSTER 17	PTA-17	Day 2 15 th Dec. 7:50 pm IST (5 minutes)
20	Aiswarya Samal Indian Institute of Technology Bhubaneswar, Odisha, India	First principles study of strain effect on thermal and electrical transport of metal and graphene	Theory Application - POSTER 18	PTA-18	Day 2 15 th Dec. 7:55 pm IST (5 minutes)
21	Prince Gollapalli Department of Metallurgical and Materials Engineering, Indian Institute of Technology, Madras, Chennai, India	On the Origin of Chemically Graded Metal/Ceramic Interface - A High Throughput DFT Study	Theory Application - POSTER 19	PTA-19	Day 3 16 th Dec. 5:00 pm IST (5 minutes)
22	V. Rajapandian Department of Chemistry, Sri Ramakrishna Mission Vidyalaya College of Arts and Science, Coimbatore- 641020, Tamil Nadu, India	Force Filed Parameters for Copper Proteins	Theory Application - POSTER 20	PTA-20	Day 3 16 th Dec. 5:05 pm IST (5 minutes)
23	Preeti Department of Physics, Panjab University, Chandigarh, India	Electronic, half-metallic and magnetic properties of bulk Co ₂ TiGe Heusler alloy	Theory Application - POSTER 21	PTA-21	Day 3 15 th Dec. 7:30 pm IST (5 minutes)
24	Rohilla Department of Physics, Panjab University, Chandigarh, India	Structural, Electronic and Elastic Properties of ScP at ambient pressure	Theory Application - POSTER 22	PTA-22	Day 3 15 th Dec. 7:35 pm IST (5 minutes)
25	Monirul Shaikh Dept. of Physics and Nanotechnology, SRM Institute of Science and Technology, KTR, Tamil Nadu, India	Defect induced ferromagnetism in a two-dimensional metal–organic framework	Theory Application - POSTER 23	PTA-23	Day 3 15 th Dec. 7:40 pm IST (5 minutes)
26	Mukaddar Sk, Dept. of Physics and Nanotechnology, SRM Institute of Science and Technology, KTR, Tamil Nadu, India	First-principles study on Cs ₂ MM'Cl ₆ [M= Cu, Ag, Au; M'= Al, Ga, In, Tl] double perovskites halides for photovoltaic applications	Theory Application - POSTER 24	PTA-24	Day 3 15 th Dec. 7:45 pm IST (5 minutes)
27	M. J. Swamynadhan Dept. of Physics and Nanotechnology, SRM Institute of Science and Technology, KTR, Tamil Nadu, India	Designing multifunctional two dimensional layered Van der Waals transition metal phosphorous chalcogenides	Theory Application - POSTER 25	PTA-25	Day 3 15 th Dec. 7:50 pm IST (5 minutes)

28	Goutam Paul, School of Physical Sciences, Indian Association for the Cultivation of Science, Kolkata, India	Structure, Morphology, and Photovoltaic Implications of Halide Alloying in Lead-Free $\text{Cs}_3\text{Sb}_2\text{Cl}_{19-x}$ 2D-layered Perovskites	Experiment -POSTER 1	PEX1	Day 5 18 th Dec. 6:00 pm IST (5 minutes)
29	Mrs. K. Safna, Govt. polytechnic College, Chelakkara, Thrissur- 680586, Kerala, India	Tailoring of optical band gap and microstructure profiling of vanadium based complex compound systems	Experiment -POSTER 2	PEX2	Day 5 18 th Dec. 6:05 pm IST (5 minutes)
30	Raja Chakraborty, School of Physical Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700032, India	Dynamic Response of Alternating-Current-Driven Light-Emitting Diodes Based on Hybrid Halide Perovskites	Experiment -POSTER 3	PEX3	Day 5 18 th Dec. 6:10 pm IST (5 minutes)
31	Pratap Pal, Indian Institute of Technology Kharagpur, West Bengal-721302, India	Towards enhanced room- temperature photovoltaic effect in ferroelectric Bi and Fe codoped BaTiO_3	Experiment -POSTER 4	PEX4	Day 5 18 th Dec. 6:15 pm IST (5 minutes)
32	Priyaath Mal Department of Pure and Applied Physics, Guru Ghasidas Vishwavidyalaya, Koni, Bilaspur-405009, India	Comparative Fermiology Study of PbBi_2Te_4 and SnBi_2Te_4 3D Topological Insulators	Experiment -POSTER 5	PEX5	Day 5 18 th Dec. 6:20 pm IST (5 minutes)