Advances in Materials Research and Simulation

Indian Association for the Cultivation of Science, Kolkata

Date : 25th May, 2018 **Venue:** C.V. Raman Hall

Materials research today has emerged as an interdisciplinary field of science with close integration of theory, computation, experiment and data science. Theoretical advances in quantum and statistical mechanical tools, backed by state-of-the-art computational techniques have pushed the frontiers of this field from 'understanding' to 'prediction' and 'discovery' of new materials with tailored physical and chemical properties. For the electronic level description of materials, the density functional theory plays a dominating role. This one-day seminar is aimed at giving some glimpses at this emerging world of materials theory and modeling, as can be seen from the topics covered both on methodologies and applications.

Program Details

10. 00 : Inaugural Session

Session I Chair : Prof. Shyamal Bhadra

10:15 – 10:45: 'Adventures in Density Functional Theory', Prof. Swapan Kumar Ghosh, DAE. Mumbai
10:45 – 11:15:'Parametric Oscillation in Chemical Systems',Prof. Deb Shankar Ray, IACS, Kolkata
11. 15 – 11. 45: 'Dichalcogenides before the recent hype', Prof. Argha Taraphder, IIT Kharagpur and IIT Mandi

11.45 – 12.00: Tea Break

Session II Chair : Prof. Kalyan K. Chattopadhyay

12:00 –12: 30 : 'Transport properties of two-dimensional Nanomaterials', Prof. Sugata Mukherjee, S.N. Bose National Centre for Basic Sciences
12:30 – 12.50: 'First principles based modelling and simulation of energy and functional materials', Dr. Satadeep Bhattacharyya, Indo-Korean Science and Technology Center, Bangalore
12:50 – 13:10: 'Functional Materials by Multimode Coupling', Dr. Saurabh Ghosh, SRM IST, Chennai

13.10 – 14.15: Lunch Break

Session III Chair : Prof. Bimalendu Deb

14. 15 – 14.45: 'Plasmon in Semiconductor Nanocrystals', Prof. Subodh K. De, IACS, Kolkata
14. 45 –15.05 : 'Heterogeneous catalyst and solar absorber materials: First-principles theoretical study' Dr. Ranjit Thapa, SRM IST, Chennai *(over Skype)*
15:05 – 15:25 : 'Theoretical evidence for unexpected O-rich phases at corners of MgO surfaces Dr. Saswata Bhatachariya, IIT Delhi
15:25 – 15.45: 'Modulating the lattice dynamics of n-type Heusler compounds via tuning Ni concentration' Dr. Amrita Bhattacharya, IIT Bombay

15.45 – 16.00 : Tea Break

Session IV Chair : Prof. Indra Dasgupta

16:00 – 17:30 p.m.: Special Session

17.30: Concluding remarks followed by High Tea.

All are cordially welcome

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Organizing Team

Dr. Saurabh Ghosh, Paramita Banerjee, Tisita Das, Moumita Mukherjee