

## **(20) Computational Materials Science**

Co-chairs

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**DETAILED PROGRAMME****Tuesday : 13-12-2016****Session I : 10.15-11.45**

10.15-10.45 Invited Talk (1)	<u>Varadharajan Srinivasan</u>	<b>ABS-Email-ICYRAM</b> Towards <i>ab initio</i> design of multiferroic double perovskite compounds
10.45-11.15 Invited Talk (2)	<u>Sandip Bhattacharya</u>	<b>ABS-Email-ICYRAM</b>
11.15-11.45 Invited Talk (3)	<u>Sudipta Dutta</u>	<b>ABS-Email-ICYRAM</b>

**Tuesday : 13-12-2016****Session II : 12.00-13.15**

12.00-12.30 Invited Talk (4)	<u>Joydeep Bhattacharjee</u>	<b>ABS-Email-ICYRAM</b> Nearest neighbour ferromagnetism in partially gated graphene
12.30-12.45 Oral (1)	<u>Shashi Bhusan Mishra</u> Somnath Chanda Roy B. R. K. Nanda	<b>ABS-232-ICYRAM</b> Adsorption of CO <sub>2</sub> on the TiO <sub>2</sub> Surface with and without a graphene overlayer: First Principle Study
12.45-13.00 Oral (2)	<u>Soorya Kabekkodu</u> Thomas Blanton Justin Blanton Timothy Fawcett	<b>ABS-336-ICYRAM</b> 75 Years of the Powder Diffraction File™: An Overview of Database Development for Materials Science and Characterization

**Tuesday : 13-12-2016****Session III : 16.00-18.00**

16.00-16.30 Invited Talk (5)	<u>Prasenjit Ghosh</u> Nandha Kumar	<b>ABS-Email-ICYRAM</b> Selectivity and Reactivity of Pd Containing Low Indexed PdGa Surfaces Towards Selective Hydrogenation of Acetylene: Interplay of Surface Roughness and Ensemble Effect
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16.30-17.00 Invited Talk (6)	Abhishek K. Singh	<b>ABS-Email-ICYRAM</b> Outlook and Challenges for Hydrogen Storage via Kubas Interaction
17.00-17.30 Invited Talk (7)	<u>Raghunathan Ramakrishnan</u>	<b>ABS-Email-ICYRAM</b>
17.30-17.45 Oral (3)	<u>S. Agrawal</u> K. Mondal, D. Manna A. Banerjee, T.K. Ghanty	<b>ABS-567-ICYRAM</b> Hydrogen doped Gold nanocluster: Isomers and chemical properties
17.45-18.00 Oral (4)	<u>R Aneela</u> V. V. S. S. Srikanth	<b>ABS-662-ICYRAM</b> Thermodynamic Study on Diamond-WC Co-formation from H <sub>2</sub> -CH <sub>4</sub> -WCl <sub>6</sub> Gas Mixture

**Wednesday : 14-12-2016**

**Session IV : 12.00-13.15**

12.00-12.30 Invited Talk (8)	<u>Ranjit Thapa</u>	<b>ABS-Email-ICYRAM</b> Identification of <b>descriptor</b> for carbon (sp <sup>2</sup> hybridized) based electrocatalyst & <b>Si doped T6</b> structure (sp <sup>2</sup> +sp <sup>3</sup> ) as anode material for <b>LiB's</b>
12.30-13.00 Invited Talk (9)	<u>Priya Johari</u>	<b>ABS-Email-ICYRAM</b> The Unexplored Thermodynamically Stable Li-Sn Compounds at Ambient and High Pressure
13.00-13.15 Oral (5)	<u>Tanmay Sarkar</u> Mridula d. Bharadwaj A. S. Prakash	<b>ABS-Email--ICYRAM</b> Oxygen stability study of Li-rich compound: First-Principles Analysis

**Wednesday : 14-12-2016**

**Session V : 14.15-15.45**

14.15-14.45 Invited Talk (10)	<u>Saswata Bhattacharya</u>	<b>ABS-Email-ICYRAM</b> Solving The "Inverse Problem" In Materials Science For Nano-Clusters: Cascade Genetic Algorithm And Beyond
14.45-15.15 Invited Talk (11)	<u>Bhalchandra Pujari</u>	<b>ABS-Email-ICYRAM</b> Ab initio method for construction of Magnetic Phase Diagram of Random Alloys

15.15-15.30 Oral (6)	<u>A. M. Dongare</u> G. Agarwal S. A. Suresh	<b>ABS-225-ICYRAM</b> Atomic Scale and Mesoscale Modeling of Metallic Materials under Mechanical Extremes
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**Wednesday : 14-12-2016**  
**Session VI : 16.00-18.00**

16.00-16.30 Invited Talk ( 12)	<u>Prabuddha Sanyal</u>	<b>ABS-301-ICYRAM</b> Novel high Tc half-metallic phases and metal-insulator transitions in 3d-5d double perovskites
16.30-17.00 Invited Talk (13)	<u>Chandan Bera</u>	<b>ABS-257-ICYRAM</b> Computational prediction of thermoelectric materials
17.00-17.15 Oral (7)	<u>S. Mitra</u> S. Chakrabarti A. Ahmad, A. K. Das	<b>ABS-234-ICYRAM</b> A First principle study of Electronic and Magnetic properties of Co <sub>2</sub> ZrZ (Z= Al ,Si, Ge) Full-Heusler Alloys
17.15-17.30 Oral (8)	<u>Saswata Halder</u> Binita Ghosh Pranay Biswas T. P. Sinha	<b>ABS-398-ICYRAM</b> Understanding the X-ray photoelectron spectroscopy and Photophysical properties of double perovskite A <sub>2</sub> SmTaO <sub>6</sub> (A= Ba, Sr, Ca) from First Principles Density Functional Theory Calculations
17.30-17.45 Oral (9)	<u>T. Premkumar</u> M Aldritt Scaria R. Vidya	<b>ABS-546-ICYRAM</b> Crystal Structure and Electronic Structure Studies on Transparent Conducting Nitrides

**Poster Session**

**Thursday : 15-12-2016 : Time : 10.15-13.15 hrs**

20-Poster-01	Bramha P. Pandey V. Kumar	<b>ABS-8-ICYRAM</b> Structural and elastic properties calculation of CdX (X= S, Se, Te) semiconductors from First-principles
20-Poster-02	Sumit Sharma Rakesh Chandra Pramod Kumar Navin Kumar	<b>ABS-13-ICYRAM</b> Effect of stone-wales and vacancy defects on elastic moduli of carbon nanotubes and their composites using molecular dynamics simulation
20-Poster-03	S. Sharma P. Kumar R. Chandra	<b>ABS-30-ICYRAM</b> Mechanical and Thermal Properties of Graphene/Carbon Nanotube Reinforced Nickel Composites: A Molecular Dynamics Study

20-Poster-04	Prakhar Gupta Ajeet Kumar	<b>ABS-108-ICYRAM</b> Unusual buckling in nanorods and nanotubes explained using Helical Cauchy Born rule
20-Poster-05	Shyam M. Keralavarma M Rajaguru	<b>ABS-193-ICYRAM</b> Mesoscale Simulation of Dislocation Creep in Single Crystals
20-Poster-06	Aniruddha Ghosh Anshul Yadav Arvind Kumar	<b>ABS-262-ICYRAM</b> Numerical Prediction of Output Responses and Microstructural Study in Submerged Arc Welding Process
20-Poster-07	I. Manjubala Nikhil Iyer Febin Rahman U.Narendra Kumar	<b>ABS-602-ICYRAM</b> Influence of structural features on mechanical performance of dental implants
20-Poster-08	J. Karthikeyan Vijay Kumar P. Murugan	<b>ABS-630-ICYRAM</b> Role of Valance Electron Concentration in Determining Structural Stability and Electronic Properties of Mo-S Nanostructures
20-Poster-09	Arunkumar Jayakumar Maximiano Ramos Ahmed Al-Jumaily	<b>ABS-751-ICYRAM</b> Correlation of Heat and Current Distribution in the GDL of a PEMFC Stack
20-Poster-10	M Vivek Ghate Shaila A Lewis Abhishek Chandra	<b>ABS-Email-ICYRAM</b> <i>In silico</i> investigation of the Inclusion Complex of $\beta$ -cyclodextrin and its derivatives with Telmisartan