

(23) Computational Materials Science

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DETAILED PROGRAMME

Monday, 16-12-2013

Session I : 11.45 – 13.15

11.45 - 12.15 Invited Talk (1)	<u>Su-Huai Wei</u>	ABS - Email - ICA Rational Design of Semiconductors for Hydrogen Production through Photoelectrochemical Water Splitting
12.15 - 12.45 Invited Talk (2)	<u>Tanusri Saha-Dasgupta</u>	ABS - Email - ICA First-principles Study of Spin-Crossover Polymers
12.45 - 13.00 Oral (1)	<u>Deepashri Saraf</u> and Anjali Kshirsagar	ABS - 345 - ICA First-principles modeling of electronic structure at nanocontacts of surface passivated CdSe nanorods with gold clusters

Session II : 16.00 – 18.00

16.00 - 16.30 Invited Talk (3)	<u>Hyuagjun Kim</u>	ABS - Email - ICA Toward a lithium 'air' battery : The effect of Co ₂ on the chemistry of a lithium-oxygen cell
16.30 - 17.00 Invited Talk (4)	<u>Chun Zhang</u>	ABS - Email - ICA Electronic and Transport Properties of Molecular Junctions under a Finite Bias: A Dual Mean Field Approach
17.00 - 17.15 Oral (2)	<u>Nisha Mammen</u> Stefano de Gironcoli Shobhana Narasimhan	ABS - 1009 - ICA Substrate Doping: A strategy for enhancing reactivity of Gold nanocatalysts by tuning <i>sp</i> -bands
17.15 - 17.30 Oral (3)	<u>A.H.M. Abdul Wasey</u> Soubhik Chakrabarty C. Majumder and G.P. Das	ABS - 1327 - ICA Substrate Induced Functionalization of Hexagonal Boron Nitride Sheet
17.30 - 17.45 Oral (4)	<u>Ranjit Thapa</u> <u>Sinthika S</u>	ABS - 1538 - ICA Au based nanoparticles as an efficient catalyst and the particular role of the surface <i>s</i> states: First-principles study

Thursday, 19-12-2013

Session III : 10.15 – 11.15

10.15 - 10.45 Invited Talk (5)	<u>Satoshi Watanabae</u> , Xiao Bo and Shusuke Kasamatsu	ABS - Email - ICA First-Principles Simulations on Electric and Dielectric Properties of Metal-Oxide Heterostructures for Novel Nanoscale Devices
10.45 - 11.00 Oral (5)	<u>Kanchan Ulman</u> Shobhana Narasimhan and Anna Delin	ABS - 1060 - ICA Tuning Spin Transport Properties and Molecular Magnetoresistance Through Contact Geometry

Session IV : 11.45 – 13.15

11.45 - 12.15 Invited Talk (6)	Tushar K. Ghosh and <u>Nisanth N. Nair</u>	ABS - Email - ICA H ₂ formation from Water at the Rh/Al ₂ O ₃ Interface
12.15 - 12.30 Oral (6)	<u>Arijit Sen</u>	ABS - 1526 - ICA Charge Transport across Nanoelectronic Devices: Electrode Morphology vs. Molecular Conformation
12.30 - 12.45 Oral (7)	Sandeep Nigam and <u>Chiranjib Majumder</u>	ABS - 1619 - ICA Structural and electronic properties of noble metal clusters on metal oxide support: Implications toward advancing the frontiers in nano catalysis

Friday, 20-12-2013**Session V : 10.15 – 11.15**

10.15 - 10.45 Invited Talk (7)	<u>Saswata Bhattacharya</u> , Sergey V. Levchenko, Luca M. Ghiringhelli, Matthias Scheffler	ABS - Email - ICA Stability and Metastability of Clusters in a Reactive Atmosphere: Theoretical Evidence for Unexpected Stoichiometries of Mg _M O _x
10.45 - 11.00 Oral (8)	<u>Joy Mitra</u> Ashok Arya and Gautam K. Dey	ABS - 622 - ICA Shockley Partial in Ordered Ni ₃ Nb (DO22) Phase – A First-Principle Study
11.00 - 11.15 Oral (9)	<u>Sananda Biswas</u> Gustav Bihlmayer Shobhana Narasimhan and Stefan Blügel	ABS - 1131 - ICA Noncollinear magnetic properties of surface-alloys on Ru(0001): A firstprinciples study

Session VI : 11.45 – 13.15

11.45 - 12.15 Invited Talk (8)	<u>Saroj K Nayak</u>	ABS - Email - ICA Predictive Large Scale Electronic Structures for Materials Design: from Nanoelectronics to Biotechnology
12.15 - 12.45 Invited Talk (9)	<u>Hongjun Xiang</u>	ABS - Email - ICA Unified model for spin order induced polarization in Multiferroics
12.45 - 13.00 Oral (10)	<u>Rajiv K. Chouhan</u> Aftab Alam Subhradip Ghosh and Abhijit Mookerjee	ABS - 1648 - ICA A first principle study of the force constants role in the lattice dynamics of disordered alloys
13.00 - 13.15 Oral (11)	<u>Tribhuwan Pandey</u> and Abhishek K. Singh	ABS - Email - ICA Role of defect transition level in tuning the thermoelectric properties of doped CrSi ₂

Poster Session :**Thursday, 19-12-2013, 14.00 to 15.30**

23 - Poster - 01	S. Sharma and Y.C. Sharma	Electronic structure study of some chalcogenide glasses	ABS - 20 - ICA
23 - Poster - 02	J. Karthikeyan Vijay Kumar and P. Murugan	Structure, Electronic and Magnetic Properties of One dimensional MoS _{2+x} NanoRibbons	ABS - 51 - ICA
23 - Poster - 03	Laxman Tatikondewar Deepashri Saraf Pravin P. Ingole Ganesh B. Markad, Omkar Nene, Santosh K. Haram and Anjali Kshirsagar	Band Gap Bowing at Nanoscale: Investigation of CdS _x Se _(1-x) Alloy Quantum Dots through Cyclic Voltammetry and Density Functional Theory	ABS - 344 - ICA
23 - Poster - 04	Alo Dutta and T. P. Sinha	Electronic structure and phonon modes of Sr ₂ SmNbO ₆	ABS - 389 - ICA
23 - Poster - 05	B. P. Pandey and V. Kumar	Structural and electronic properties of In _x Ga _{1-x} As alloy using First Principles	ABS - 524 - ICA
23 - Poster - 06	S. Seenithurai R. Kodi Pandyan S. Vinodh Kumar C. Saranya and M. Mahendran	Hydrogen Storage in Graphene Functionalized with Alkali Metals	ABS - 838 - ICA
23 - Poster - 07	R. Kodi Pandyan S. Seenithurai S. Vinodh Kumar C. Saranya and M. Mahendran	Transition Metal Hydride Doped SWCNT for Hydrogen Adsorption	ABS - 838a - ICA
23 - Poster - 08	S.G. Khambholja B.Y. Thakore P.N. Gajjar and A.R. Jani	High Pressure Melting Curve of Lithium Fluoride	ABS - 858 - ICA
23 - Poster - 09	E.Shama Pearlin V.Krishnakumar and R.Nagalakshmi	Studies on 7-[(Morpholin-4-yl)(phenyl)methyl]quinolin-8-ol	ABS - 923 - ICA
23 - Poster - 10	Sukanya Ghosh Nisha Mammen and Shobhana Narasimhan	Tuning the properties of oxide substrates used in catalysis, by anion doping	ABS - 978 - ICA
23 - Poster - 11	M. K. Singh Rachna Selvamani Gurvinderjit Singh and V. S. Tiwari	Local Atomic Structure of Na _{0.5} Bi _{0.5} TiO ₃ using Raman Scattering Study	ABS - 1044 - ICA

23 - Poster - 12	Rajdeep Banerjee Sukanya Ghosh Nisha Mammen Aruna Nair and Shobhana Narasimhan	The unsuspected role of <i>s</i> - and <i>p</i> -electrons in the reactivity of gold nanoparticles	ABS - 1064 - ICA
23 - Poster - 13	Vasudevan. M. V Shobhana Narasimhan	Mixed Self Assembled monolayers for modulation of work function of Au(111) surface	ABS - 1132 - ICA
23 - Poster - 14	Debdipto Acharya Sananda Biswas and Shobhana Narasimhan	H ₂ adsorption on pristine and doped hexagonal Boron Nitride (h-BN) sheet	ABS - 1165 - ICA
23 - Poster - 15	Krushna M Mohapatra and Birendra Panda	Many-Body Theory of Dark Current in Quantum Well Based Infrared Photodetector	ABS - 1274 - ICA
23 - Poster - 16	Narayan C. Bera	Ion Energetics Properties of VX: Theoretical and CIMS study	ABS - 1691 - ICA