Electronic structure approaches to Atoms, Molecules, Clusters and Solids (7-11, January 2013)
Advanced Centre of Research in High Energy Materials, University of Hyderabad

Patron:

Prof. Ramakrishna Ramaswamy (Vice-chancellor, University of Hyderabad)

Organisers:

G. S. Vaitheeswaran
Advanced Centre of Research in High Energy Materials (ACRHEM)
University of Hyderabad

Director, ACRHEM, University of Hyderabad

Prof. Surya P. Tewari
School of Physics and ACRHEM
University of Hyderabad

Objective of the Meeting

- To provide a platform for discussion and expose young researchers to the field of electronic structure calculations.
- Applications of electronic structure methods in physics, chemistry, engineering and technology.

About the Meeting

The meeting is so designed that the participants would learn the fundamental aspects of electronic structure methods from the experts and from the academia. Participants will get opportunity to get familiarized on the advances in density functional theory (DFT) and on various DFT codes used to study the physical and chemical properties of atoms, molecules, clusters and solids.

Topics covered

- Basics of density functional theory
- Fundamentals of electronic structure methods
- Design and study of high energy materials (HEMs)

- Physics and chemistry of atoms, molecules and clusters of hydrides.
- Mechanical, optical, and thermodynamic properties of materials.
- Magnetic and superconducting materials
- Low dimensional systems
- van der Waals corrected density functional theory
- Hydrogen Storage
- Excited state study of molecules
- Clusters
- Physics and chemistry of Rare-earth and Actinides
- High-pressure studies

Local Organizing Committee:

Prof. S. Mahapatra
Dr. A. K. Chaudhary
Dr. S. Venugopal Rao
Dr. Prem Kiran
Dr. G. Manoj Kumar
Prof. K. C. James Raju
Prof. M. Ghanshyam Krishna
Mr. Sadik Hussain

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S. D. Mahanti (Michigan State University, USA)

Sashi Satpathy (University of Missouri, Columbia, USA)

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Swapan K. Ghosh (BARC, Mumbai)

Tanusri Saha Dasgupta (SNBNCBS, Kolkata)

Umesh V. Waghmare (JNCASR, Bangalore)

International Speakers: (Confirmed list)

Axel Svane (Aarhus University, Denmark)

Biplab Sanyal (Uppsala University, Sweden)

Dasari Prasad (Cornell University, USA)

N. E. Christensen (Aarhus University, Denmark)

Priya Vashishta (University of South California, LA, USA)

Puru Jena (Virginia Commonwealth University, Richmond, USA)

Ralph Scheicher (Uppsala University, Sweden)

S. D. Mahanti (Michigan State University, USA)

Sangeeta Sharma (MPI, Halle, Germany)

Saroj K. Nayak (Rensselaer Polytechnic Inst., USA)

Sébastien Lebégue (CNRS, Nancy, France)

S. Shallcross (Institute für Technische Physik III, Erlangen, Germany)

National Speakers (Confirmed list)

Abhishek K. Singh (IISC, Bangalore)

Ayan Datta (IACS, Kolkatta)

D. D. Sarma (IISc, Bangalore)

D. G. Kanhere (Central Univ. of Rajasthan, Rajasthan)

G. P. Das (IACS, Kolkata)

G. Baskaran (IMSC, Chennai)

G. Narahari Sastry (IICT, Hyderabad)

Indra Dasgupta (IACS, Kolkata)

K. R. S. Chandrakumar (BARC, Mumbai)

Kalidas Sen (UoH, Hyderabad)

Kalobaran Maiti (TIFR, Mumbai)

Manoj K. Harbola (IIT Kanpur)

M. C. Valsa Kumar (IGCAR & University of Hyderabad)

Mrinilalini Deshpande (H. P. T. Arts and R.Y. K. Science college, Nasik)

Pratim Kumar Chattaraj (IIT, Kharagpur)

Presenjit Sen (HRI, Allahabad)

Priya Mahadevan (SNBNCBS, Kolkata)

R. Prasad (IIT, Kanpur)

Shobhana Narasimhan (JNCASR, Bangalore)

Sourav Pal (NCL, Pune)

Subhradip Ghosh (IIT, Guwahati)

Sushil Auluck (NPL, New Delhi)

Swapan K. Ghosh (BARC, Mumbai)

Tanusri Saha Dasgupta (SNBNCBS, Kolkata)

V. Kanchana (IIT, Hyderabad)

Vijay Kumar (Vijay Kumar Foundation, Gurgaon)

Electronic Structure Approaches to Atoms, Molecules, Clusters and Solids

(07th -11th January 2013 at University of Hyderabad, Hyderabad)

Schedule of talk

Date & Time	Speaker	Title
07th Jan 2013 08:00 – 09:00 a.m.	Registration	Venue: ACRHEM, South Campus, University of Hyderabad
07th Jan 2013 09:00 - 09:30 a.m.	**Prof. R. Ramaswamy** Hon. Vice Chancellor University of Hyderabad	Inauguration/Inaugural Address
07th Jan 2013 09:30 - 10:15 a.m.	**G. Baskaran** IMSc, Chennai	Superradiant Superconductivity - a Novel Electronic State
07th Jan 2013 10:15 - 10:45 a.m.	High Tea	
07th Jan 2013 10:45 – 11:30 a.m.	**Puru Jena** Virginia Commonwealth University, Richmond, USA	Beyond The Periodic Table: Role of Clusters
07th Jan 2013 11:30 – 12:15 p.m.	**Shobhana Narasimhan** JNCASR, Bangalore	Tuning the morphology and reactivity of gold clusters by substrate doping
07th Jan 2013 12:15 – 01:00 p.m.	**D. G. Kanhere** Central University of Rajasthan, Rajasthan	Dynamics of glass forming clusters
07th Jan 2013 01:00 - 02:00 p.m.	Lunch	
07th Jan 2013 02:00 - 02:45 p.m.	**Biplab Sanyal** Uppsala University, Sweden	Functionalization of graphene and graphene oxide by organic molecules
07th Jan 2013 02:45 – 03:30 p.m.	**Ralph H. Scheicher** Uppsala University, Sweden	DNA sequencing with graphene nanopores explored using *ab initio* methods
07th Jan 2013 03:30 - 04:00 p.m.	Tea	
07th Jan 2013 04:00 - 04:45 p.m.	**G. P. Das** IACS, Jadavpur, Kolkata	Can nanostructures be functionalized for efficient storage of hydrogen?
07th Jan 2013 04:45 – 05:30 p.m.	**Dasari L. V. K. Prasad** Cornell University, USA	Electronic structure and dynamics of H/Li/N systems at high pressure
08-01-2013		
08th Jan 2013 09:00 - 09:45 a.m.	**S. D. Mahanti** Michigan State University, Michigan, USA	Bands, Band gaps and Thermoelectric properties of Ternary Diamond-like Semiconductors
08th Jan 2013 09:45 – 10:30 a.m.	**Sushil Auluck** NPL, Delhi	Thermoelectrics at CSIR@NPL
08th Jan 2013 10:30 – 10:45 a.m.	Tea	
08th Jan 2013 10:45 – 11:30 a.m.	**Priya Vashishta** University of Southern California, USA	Reactive Nanosystems: Multimillion Atom Molecular Dynamics Simulations of Energetic Materials
08th Jan 2013 11:30 - 12:15 p.m.	**Saroj K. Nayak** IIT Bhubaneshwar and Rensselaer Polytechnic Inst., USA	Large Scale Electronic Structure and Quantum Transport at Nanoscale
08th Jan 2013 12:15 – 01:00 p.m.	**R. Prasad** IIT Kanpur, Kanpur	Electronic Structure of Topological Insulators
08th Jan 2013 01:00 - 02:30 p.m.	Lunch	

08th Jan 2013 02:30 – 04:00 p.m.	Poster Session	
08th Jan 2013 04:00 – 04:30 p.m.	Tea	
08th Jan 2013 04:30 – 05:30 p.m.	**D. D. Sarma** IISc Bangalore	Special Evening Lecture Title: Electronic structure of transition metal oxides (and some more)
09-01-2013		
09th Jan 2013 09:00 - 09:45 a.m.	**Manoj K. Harbola** IIT Kanpur	Band-gap problem in density-functional theory (DFT)
09th Jan 2013 09:45 – 10:30 a.m.	**Indra DasGupta** IACS, Jadavpur, Kolkata	Electronic structure and novel functionalities in low dimensional and cluster assembled solids.
09th Jan 2013 10:30 – 10:45 a.m.	Tea	
09th Jan 2013 10:45 – 11:30 a.m.	**Sangeeta Sharma** MPI Halle, Germany	Excitons in solids captured with bootstrap approximation for the exchange-correlation kernel of time-dependent density functional theory
09th Jan 2013 11:30 – 12:15 p.m.	**Sebastien Lebègue** CNRS, France	Van der Waals forces in solids: semi-empirical and ab-initio calculations
09th Jan 2013 12:15 – 01:00 p.m.	**Tanusri Saha-Dasgupta** SNBNCBS, Kolkata	First-principles Study of Spin-Crossover Polymers
09th Jan 2013 01:00 – 02:15 p.m.	Lunch	
09th Jan 2013 02:15 – 03:00 p.m.	**S. Shallcross** Institut für Technische Physik III, Erlangen, Germany	Localisation and van Hove singularities in the graphene twist bilayer
09th Jan 2013 03:00 – 03:45 p.m.	**Swapan K Ghosh** BARC, Mumbai	Chemistry of Molecules to Physics of Materials: A Unified View through Density Window
09th Jan 2013 03:45 – 04:15 p.m.	Tea	
09th Jan 2013 04:15 – 05:00 p.m.	**P. K. Chattaraj** IIT Kharagpur	All-metal Aromaticity and Conceptual DFT
09th Jan 2013 05:00 – 05:45 p.m.	**Subhradip Ghosh** IIT Guwahati	Effects of chemical disorder on magnetic properties of potential shape memory alloys in Heusler and Inverse Heusler structures
10-01-2013		
10th Jan 2013 09:00 – 09:45 a.m.	**Niels E. Christensen** Aarhus University, Denmark	Electronic quasiparticle states of PbX (X=S,Se,Te) and SnTe.
10th Jan 2013 09:45 – 10:30 a.m.	**Axel Svane** Aarhus University, Denmark	Quasi particle self-consistent GW calculations for Actinides and Hg semiconductors
10th Jan 2013 10.30 - 11.00 a.m.	Tea	
10th Jan 2013 11:00 – 11:45 a.m.	**Mrinalini Deshpande** H.P.T. Arts and R.Y.K. Science College, Nasik	Structural and Electronic Properties of Yttrium/Gadolinium-Doped Alumina Clusters : First Principles Calculations
10th Jan 2013 11:45 - 12:30 p.m.	**Kalobaran Maiti** TIFR, Mumbai	Electronic structure of Fe-superconductors
10th Jan 2013 12:30 - 02:00 p.m.	Lunch	
10th Jan 2012 02:00 – 02:45 p.m.	**Prasenjit Sen** HRI, Allahabad	Electronic structure of TM-Sr clusters: Are there new magnetic superatoms?
10th Jan 2013 02:45 – 03:30 p.m.	**Vijay Kumar** Shiv Nadar University, Uttar Pradesh	Magnetism in Doped Clusters of Gold and Compound Semiconductors
10th Jan 2013 03:30 – 04:00 p.m.	Tea	

10th Jan 2013 04:00 – 04:45 p.m.	**Abhishek K. Singh** IISc, Bangalore	Effect of Normal Strain on Electronic Properties of few layers of MoS_2
10th Jan 2013 04:45 – 05:30 p.m.	**Priya Mahadevan** SNBNCBS, Kolkata	A route to high Neel temperatures in 4d and 5d transition metal oxides
11-01-2013		
11th Jan 2013 09:00 - 09:45 a.m.	**K. D. Sen** University of Hyderabad	Scaling properties of net information measures and statistical complexity for bound states of spherical model potentials
11th Jan 2013 09:45 – 10:30 a.m.	**Sourav Pal** NCL, Pune	Metals and metal-organic frameworks as materials for catalysis and reversible hydrogen storage: Computational study
11th Jan 2013 10.30 - 11.00 a.m.	Tea	
11th Jan 2013 11:00 – 11:45 a.m.	**Ayan Datta** IACS, Kolkata	Silicene: Its different from Graphene
11th Jan 2013 11:45 - 12:30 p.m.	**G. Narahari Sastry** IICT, Hyderabad	Understanding the Formation of Macromolecular Assemblies: A Structural Perspective
11th Jan 2013 12:30 – 02:00 p.m.	Lunch	
11th Jan 2013 02:00 – 02:30 p.m.	**V. Kanchana** IIT Hyderabad	Fermi Surface topology change in Superconducting Intermetallics under pressure
11th Jan 2013 02:30 – 03:00 p.m.	**K. R. S. Chandrakumar** BARC, Mumbai	Nucleation and Growth Mechanism of Carbon Nanotubes: Insights from DFTB based QM/MD Simulations
11th Jan 2013 03:30 – 04:00 p.m.	**M . C. Valsa Kumar** IGCAR / University of Hyderabad	
11th Jan 2013 04:00 – 04:30 p.m.	Concluding Session (Remarks/Comments)	