

Programme Schedule of ATHENA 2012

Venue: Fermion, S.N. Bose Centre

Monday, April 09, 2012

8:45 –9:30 Registration

9:30 – 9:45 Inauguration

Session1: Overview of Oxides :- Chair : Prof. A. K. Raychaudhuri

9.45 – 10.45 Igor Solovyev

Magnetic, orbital, and charge ordering in complex oxides I

10.45 – 11.15 Tea

11.15 – 12.45 Josep Fontcuberta

Surfaces and interfaces in oxides.

12.45 – 13.00 K. Manna

Experimental Evidences for the Spin-glass ground state in $La_{0.85}Sr_{0.15}CoO_3$ single crystals.

13.00 – 14.00 Lunch (Venue: Krishnachura hostel complex)

Session2: DFT and beyond :- Chair: Prof. G. P. Das

14.00 – 15.00 Stefano Sanvito

A rough guide to Density Functional Theory.

15.00 – 16.00 Alessio Fillipetti

A novel self-interaction correction based functional for correlated oxides: method description and applications

16.00 – 17.00 Tea + Poster (Posters will be displayed on all days)

17.00 – 18.00 Cesare Franchini

Introduction to Hybrid Functionals: theory and applications

19.30 onwards Banquet at Krishnachura hostel complex

Tuesday, April 10, 2012

Session3: Excited states-I :- Chair: Prof. Abhijit Mookerjee

09.30 – 10.30 Kalobaran Maiti

Electronic structure of transition metal oxides - a photoemission study.

10.30 – 11.00 Tea

11.00 – 11.45 Silke Biermann

An Introduction to Dynamical Mean Field Theory-I

11.45 – 12.45 Pinaki Majumdar

Probing thermal effects in correlated systems.

12.45 – 13.00 Rajarshi Tiwari

Incommensurate Magnetic Order and Mott Transitions in Hubbard Model on Anisotropic Triangular Lattice

13.00 – 14.00 Lunch (Venue: Krishnachura hostel complex)

Session4: Excited State-II :- Chair: Prof. Sugata Mukherjee

14.00 – 15.00 Siddhartha Lal

Low-temperature orbital ordering and dynamical frustration of spins in $KCuF_3$.

15.00 – 16.00 C. D. Hu

The Dzyaloshinskii-Moriya interaction in metals

16.00 – 16.30 Tea

16.30 – 17.30 Subhro Sen Gupta

An introduction to Non-resonant Inelastic X-ray Scattering (NIXS) - a versatile tool to study the electronic structure of complex oxides.

Wednesday April 11, 2012

Session5: From DFT to model Hamiltonian-I :- Chair: Dr. Tom Archer

- 09.30 – 10.30** **Roman Kovacik**
Calculation of low energy model Hamiltonian parameters using Wannier Functions.
- 10.30 – 11.00** **Tea**
- 11.00 – 12.00** **Tanusri Saha Dasgupta**
Electronic Structure of Complex Materials: from First-principles study to Materials Modeling.
- 12.00 – 13.00** **Silke Biermann**
An Introduction to Dynamical Mean Field Theory-II
- 13.00 – 14.00** **Lunch (Venue: Krishnachura hostel complex)**

Session6: DFT to model Hamiltonian-II :- Chair: Prof. G.Y. Guo

- 14.00 – 15.00** **Igor Solovyev**
Magnetic, orbital, and charge ordering in complex oxides II
- 15.00 – 15.30** **Tea**
- 15.30 – 16.30** **Priya Mahadevan**
How do we understand magnetism in various transition metal oxides?
- 16.30 – 17.30** **Umesh Waghmare**
Multi-scale Modelling of Ferroelectrics: A First-principles Landau-Ginzburg Theory of Domains and Phase Transitions

Thursday April 12, 2012

Session7: Phenomena in Oxides :- Chair: Prof. Cesare Franchini

09.30 – 10.30 **Indra Dasgupta**

Strongly Correlated Systems: Role of Spin Orbit Interactions

10.30 – 11.00 **Tea**

11.00 – 12.00 **Sugata Ray**

Deceptive disorders and incomplete understanding: How far our assumptions are valid regarding the ionic distributions in Solids?

12.00 – 13.00 **Anna Roig**

Engineering iron oxide nanoparticles for theranostic (therapeutic and diagnosis) applications in nanomedicine

13.00 – 14.00 **Lunch (Venue: Krishnachura hostel complex)**

Session8:Phenomena in Oxides :- Chair: Prof. Alessio Filippetti

14.00 – 14.15 **Nirmal Ganguly**

Predicting the structure and magnetic ground states of the 3d¹ perovskite oxides SrVO₃, CaVO₃, LaTiO₃, and YTiO₃ from ab initio calculations.

14:15– 14:30 **Pramod Varma**

Density Functional Theory Studies of electrons and phonons in pyrochlores.

14.30 – 15.30 **G.Y.Guo**

Ab Initio Studies of Electronic Structure, Magnetism and Ferroelectricity in BiMnO₃ and Li(Na)Cu₂O₂.

15.30 – 16.00 **Tea**