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 – 11.15 **Josep Fontcuberta**

Surfaces and interfaces in oxides

11.15 – 11:45 **Tea**

11.45 – 12.45 **Igor Solovyev**

Magnetic, orbital, and charge ordering in complex oxides I

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 – 15.30 **Stefano Sanvito**

A rough guide to Density Functional Theory & an Introduction to hybrid functionals

15.30 – 16.30 ***Tea + Poster (Posters will be displayed on all days)***

16.30 – 17.30 **Alessio Fillipetti**

A novel self-interaction correction based functional for correlated oxides: method description 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: Dr. Tom Archer

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: Prof. Sugata Mukherjee

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

<u>Session7: Phenomena in Oxides :-</u> Chair: Prof.Stefano Sanvito

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)

<u>Session8:Phenomena in Oxides :-</u> Chair: Prof. Alessio Filippetti

14.00 – 14.15 Nirmal Ganguly

Predicting the structure and magnetic ground states of the $3d^1$ perovskite oxides $SrVO_3$, $CaVO_3$, $LaTiO_3$, and $YTiO_3$ 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 $BiMnO_3$ and $Li(Na)Cu_2O_2$.

15.30 – 16.00 T. Archer

Multiferroic tunnel junctions from first-principles

16.00 – 16.30 Tea