

ELECTRONIC STRUCTURE : THEORY AND APPLICATIONS

Monday 14 January, 2008

- 8.30–10.30 M.K. Harbola (IITK) *Density Functional Theory*
- 10.30–11.00 COFFEE
- 11.00–13.00 O.K. Andersen (Stuttgart) *Muffin-tin Orbitals method*
- 13.00–14.00 LUNCH
- 14.00–15.00 Olle Eriksson (Uppsala) *Full-potential Linear Muffin-tin Orbitals method*
- 15.00–15.30 TEA
- 15.30–19.00 Olle Eriksson, Per Andersson (Uppsala) *FP-LMTO(RSPt): How to do it ?*

Tuesday 15 January, 2008

- 8.30–10.30 Dilip G Kanhere (Pune) *Quantum Dots and Configuration interactions*
- 10.30–11.00 COFFEE
- 11.00–13.00 Lars Nordstrom (Uppsala) *Full-potential Linear Augmented Plane Waves method*
- 13.00–14.00 LUNCH
- 14.00–19.00 Olle Eriksson, Per Andersson, Oscar Granas (Uppsala) *Hands on session on Full-potential Linear Muffin-tin Orbitals method*

Wednesday 16 January, 2008

- 8.30– 9.30 A. Mookerjee (SNBNCBS) *Real Space techniques for Electronic Structure*
- 9.30–10.30 Shobhana Narasimhan (JNCASR) *Pseudopotentials and Plane wave methods*
- 10.30–11.00 COFFEE
- 11.00–13.00 Shobhana Narasimhan (JNCASR) *Pseudopotentials and Plane wave methods*
- 13.00–14.00 LUNCH
- 14.00–19.00 *Hands on session on Pseudopotentials*

Thursday, 17 January, 2008

10.15-11.00 Debashish Mukherjee ***Treatment of dynamical and non dynamical correlations in quasi degenerate electronic states.***

11.00-11.30 COFFEE

Chairperson : B N Dev

11.30-12.15 S.P. Bhattacharyya ***Exploring soft computing methods for handling problems relating to electronic structure calculations***

12.15-13.00 A. Shukla ***Wannier function based ab initio methods for correlated calculations of dielectric response properties of solids***

13.00-14.30 LUNCH

Chairperson : Olle Eriksson

14.30-15.15 D.D.Sarma ***Magnetic and electronic structure of diluted magnetic semiconductors***

15.15-16.00 Manoj K Harbola ***Excited State Density Functional Theory***

16.00-16.30 TEA

Chairperson : Monika Mukherjee

16.30-17.15 Anna Delin ***Emerging nanomagnetic phenomena in palladium and platinum nanowires.***

17.15-18:00 G.P. Das ***Electronic Structure and Magnetism in transition metal doped semi-conducting nano-structures***

Friday 18 January, 2008

Chairperson : Ranjan Chaudhury

9.00-9.40 Lars Nordstrom ***An EXCITING Story about the APW-like method***

9.40-10.20 T. Saha-Dasgupta ***Ab-initio Study of Low dimensional quantum spin systems.***

10.20-11.00 Per Anderssen ***RSPT and f-electrons***

11.00-11.30 ***COFFEE***

Chairperson : Rajendra Prasad

11:30-12.10 A. Mookerjee ***Relativistic ASR : application to CoPt and FePd***

12.10-12.50 Sergei Simak ***Clean Air, Green Energy and First Principles Simulations***

12.50-13.30 Shobhana Narasimhan ***To Be Announced***

13.30-14.30 ***LUNCH***

Chairperson : A.K. Majumdar

14.30-15.10 Indra Dasgupta ***Magnetism in low dimensional oxides: A perspective from first principles calculations.***

15.10-15.50 Biplab Sanyal ***First Principles Modeling of Multiferroic materials.***

15:50 : ***CONCLUDING REMARKS AND COFFEE***