

**MASTANI SUMMER SCHOOL
IISER PUNE, INDIA
June 30 – July 12, 2014
Venue: Lecture Hall Complex
Program Schedule**

June 29

19:00-19:55 *Registration*

20:00 Dinner

June 30

7:00-8:00 Breakfast

8:00-9:00 *Registration*

9:00-9:45 *Inauguration*

9:45-10:15 Tea break

10:15-11:30 *Modeling materials using density-functional theory and digital computers: the plane-wave pseudopotential way* (Stefano Baroni, SISSA, Italy)

11:30-11:55 Tea break

12:00-13:00 *Doing simple calculations with Quantum ESPRESSO* (Shobhana Narasimhan, JNCASR, India)

13:00-14:25 Lunch

14:30-16:00 *Hands On: scf, Energy bands, and eqn of state* (Madhura Marathe, ETH Zurich, Switzerland)

16:00-16:30 Tea break

16:30-18:00 *Hands on contd....*

19:30 Dinner

July 1:

7:30-8:55: Breakfast

9:00-9:45 *Pseudopotentials* (Shobhana Narasimhan, JNCASR, India)

10:00-10:30 *Brillouin zone sampling, Metals and Smearing* (Shobhana Narasimhan, JNCASR, India)

10:30-11:00 Tea break

11:00-12:00 *Exchange correlation & hybrid functionals* (Stefano de Gironcoli, SISSA, Italy)

12:00-14:00 Lunch

14:00-16:00 *Hands on: scf, dos, energy bands for Al, Cu calculations* (Madhura Marathe, ETH Zurich, Switzerland)

16:00-16:30 Tea break

16:30-18:00 *Hands on: scf, dos, energy bands for Al, Cu calculations* (Madhura Marathe, ETH Zurich, Switzerland)

18:30-19:30 *Cultural program*

20:00 Dinner

July 2:

7:30-8:55: Breakfast

9:00-10:30: *Forces, stress; Atomic and cell optimizations* (Stefano de Gironcoli, SISSA, Italy)

10:30-11:00 Tea break

11:00-11:45 *The Importance of Being the Right Shape: Interplay of Geometric and Electronic Structures in Atomic Clusters* (Prasenjit Sen, HRI, India)

12:00-14:00 Lunch break

14:00-15:30 *Hands on: Geometry, cell optimization* (Madhura Marathe, ETH Zurich, Switzerland)

15:30-16:00 Tea break

16:00-17:30 *Hands on continued*

18:00-19:30 *Poster Session*

19:30 Dinner

July 3:

7:30-8:55: Breakfast

9:00-10:00 *Magnetism in DFT: from theory to practice - Part I* (Cyrille Barreteau, CEA Saclay, France)

10:00-10:30 Tea Break

10:30-11:30 ***Magnetism in DFT: from theory to practice - Part II*** (Cyrille Barreateau, CEA Saclay, France)

11:30-12:15 ***Electronic Structure of Novel Magnetic Systems: Insights from Spin-Polarized Density Functional Theory Calculation*** (Indra Dasgupta, IACS, India)

12:15-13:00 ***Spin polarized electron scattering: A method to probe magnetism at surfaces*** (P. S. Anilkumar, IISc, India)

13:00-14:30 Lunch break

14:30-16:00 ***Hands on magnetism*** (Cyrille Barreateau, CEA Saclay, France)

16:00-16:30 Tea break

16:30-18:00 ***Hands on session contd.....***

19:30 ***Conference Dinner***

July 4:

7:30-8:55: Breakfast

9:00-10:30 ***Corrections to xc functionals for strongly correlated systems: DFT+U*** (Matteo Cococcioni, EPFL Lausanne, Switzerland)

10:30-11:00 Tea break

11:00-11:45 ***Strongly correlated electrons: LDA+U in practice*** (Tanusri Saha-Dasgupta, SNBNCBS, India)

12:00-14:00 Lunch break

14:00-15:30 ***Hands on DFT+U*** (Matteo Cococcioni, EPFL Lausanne, Switzerland)

15:30-16:00 Tea break

16:00-18:00 ***Hands on session contd.....***

19:30 Dinner

July 5:

7:30-8:55: Breakfast

9:00-10:45 ***Classical MD, Ab-initio MD, CPMD*** (Dilip G. Kanhere, Univ. of Pune, India)

10:45-11:15 Tea break

11:15-12:00 ***Thermodynamic of clusters using multiple histogram method***
(Dilip Kanhere, Univ. of Pune, India)

12:00-12:30 ***Poster prize award***

12:30-14:00 Lunch break

14:00-15:30 ***Hands on*** (Vardharajan Srinivasan, IISER Bhopal, India and
Madhura Marathe, ETH Zurich, Switzerland)

15:30-16:00 Tea break

16:00-17:30 ***Hands on session contd.....***

19:30: Dinner

July 6:

Break

06:30-19:00 ***Excursion to Tamhini-Dongarwadi***

19:30 Dinner

July 7:

7:30-8:55 Breakfast (Only for registered participants)

9:00-10:30 ***TDDFT: Basics + Lancoz + Davidson*** (Ralph Gebauer, ICTP, Italy)

10:30-11:00 Tea break

11:00-11:45 ***Optical absorption spectra of chromophores in solution: the role of the solvent*** (Ralph Gebauer, ICTP, Italy)

12:00-14:00 Lunch break

14:00-15:30 ***Hands on*** (Ralph Gebauer, ICTP, Italy and Subrahmanyam Sappati,
IISER Pune, India)

15:30-16:00 Tea break

16:00-17:30 ***Hands on session contd.....***

17:30-18:00 Tea break

18:00-19:00 ***Electron correlation in excited states: Challenges to the electronic structure theories*** (Sourav Pal, CSIR-NCL, India)

19:30 Dinner

July 8:

7:30-8:55: Breakfast

9:00-10:00 ***The GW approximation*** (Manish Jain, IISc., India)

10:00-10:15 Short tea-break

10:15-11:00 ***Defects in materials*** (Manish Jain, IISc., India)

11:00-11:30 Tea break

11:30-12:30 ***Introduction to GW in QE: the GWW code*** (Margherita Marsili, University of Padova, Italy)

12:30-14:00 Lunch break

14:00-16:00 ***Hands on*** (Margherita Marsili, University of Padova, Italy)

16:00-16:30 Tea break

16:30-18:00 ***Hands on session contd.....***

19:30 Dinner

July 9:

7:30-8:55 Breakfast

9:00-10:30 ***First-principles Determination of Phonons and Related Properties*** (Umesh V Waghmare, JNCASR, India)

10:30-11:00 Tea break

11:00-11:45 ***Phonons and Related Phenomena in Materials*** (Umesh V Waghmare, JNCASR, India)

12:00-14:00 Lunch break

14:00-16:00 ***Hands on*** (Sharmila Shirodkar, JNCASR, India)

16:00-16:30 Tea break

16:30-18:00 ***Hands on session contd.....***

19:30 Dinner

July 10:

7:30-8:55: Breakfast

9:00-10:00 *Theory of Berry phases for Bloch states: Polarization and more*
(David Vanderbilt, Rutgers University, USA)

10:00-10:45 *Ferroaxial Multiferroics: A novel combination of Magnetic and Polar Order*
(Sunil Nair, IISER Pune, India)

10:45-11:15 Tea break

11:15-12:15 *Topological insulators and the quantum anomalous Hall state*
(David Vanderbilt, Rutgers University, USA)

12:15-14:15 Lunch break

14:15-15:30 *Hands on* (Sharmila Shirodkar, JNCASR, India)

15:30-16:00 Tea break

16:00-17:30 *Hands on session contd.....*

19:30 *Conference Dinner*

July 11:

7:30-8:55 Breakfast

9:00-10:30 *Vibrational Spectroscopy via Computer Simulations: Raman, Infra-Red and Related Methods*
(Ari Seitsonen, University of Zurich, Switzerland)

10:30-11:00 Tea break

11:00-11:45 *Applications of Raman in MOFs, Multiferroics and Proteins*
(Chandrabhas Narayan, JNCASR, India)

12:00-14:00 Lunch break

14:00-15:30 *Hands on* (Ari Seitsonen, University of Zurich, Switzerland)

15:30-16:00 Tea break

16:00-18:00 *Hands on session contd.....*

19:30 Dinner

July 12:

7:30-8:55 Breakfast

9:00-10:30 ***Use of QE in HPC: trend in technology for HPC, basics of parallelism and performance features*** (Ivan Girotto, ICTP, Italy)

10:30-11:00 Tea break

11:00 - 11:45 ***Use of GPU based HPC in Material Simulations*** (Ananda Bhattacharjee, NVIDIA, India)

11:45-12:30 ***Use of QE in HPC: overview of implementation and usage of the QE-GPU*** (Ivan Girotto, ICTP, Italy)

12:30-14:00 Lunch break

14:00-15:30 ***Hands on session*** (Ivan Girotto, ICTP, Italy)

15:30-16:00 Tea break

16:00-17:30 ***Hands on session contd.....***

17:45-18:00 ***Concluding remarks***

19:30 Dinner

PS: Breakfast, Lunch and Dinner will be served in the canteen in HR-4. Breakfast, lunch, dinner and conference dinners are only for registered participants and will be served only against meal coupons/invitation cards.