



The Abdus Salam  
International Centre  
for Theoretical Physics  
50th Anniversary 1964–2014



## MASTANI: Summer School on Materials Simulations Theory And Numerics 30 June – 12 July 2014

(Pune, India)

The Abdus Salam International Centre for Theoretical Physics, jointly with the Indian Institute of Science Education and Research (IISER) Pune is organizing a *Summer School on Materials Simulations Theory And Numerics* to be held in Pune, India from 30 June to 12 July 2014.

*In the proposed school we plan to cover ground state density functional theory (DFT) as well as advanced techniques. DFT has become an important tool in the area of materials research, to understand properties of materials, to complement/understand experimental results, and design new materials.*

The school is divided into two weeks. The first week is intended for all participants, and will cover the following topics:

- ✓ Basics of ground state DFT and Kohn-Sham equations
- ✓ Pseudopotentials
- ✓ Structural optimization
- ✓ Hybrid functionals
- ✓ Spin polarization including non-collinear magnetism and spin-orbit interactions
- ✓ DFT+U
- ✓ *Ab initio* molecular dynamics

The second week of the school will be restricted to participants with considerable prior experience with DFT calculations, and will cover the following topics:

- ✓ Density functional perturbation (DFPT) theory
- ✓ Time dependent DFT
- ✓ GW approximation
- ✓ Berry phase and modern theory of polarization
- ✓ Computational Infrared and Raman Spectroscopy
- ✓ Efficient use of HPC and Parallelization

*The morning sessions of the school will consist of lectures on the basic principles and methodologies followed by research talks (covering experimental and theoretical aspects) showing their applications. The afternoon sessions will consist of hands-on tutorials where the participants will do simple calculations using the Quantum ESPRESSO distribution*

### Participation

Applicants from all countries that are members of the United Nations, UNESCO or IAEA may attend. As the Workshop will be conducted in English, participants should have an adequate working knowledge of this language. The school is open to Ph D. students, Post-docs and young researchers from all countries, which are members of the United Nations, UNESCO, or IAEA. The principal objective of the Centre is to help researchers from developing countries through a programme of training activities within a framework of international cooperation. As a rule, travel and subsistence expenses of the participants should be borne by their home institutions. Every effort should be made by candidates to secure support for their fare (or at least half-fare). However, limited funds are available for some participants, who are nationals of, and working in, a developing country. Such support is available only to those who are below 35 years of age and attending the entire activity. ***In order to be eligible for the second part of the school, the participants should have proven expertise in basic DFT. There is no registration fee.***

### HOW TO APPLY FOR PARTICIPATION

The Online Application can be accessed at the activity website: <http://agenda.ictp.it/smr.php?2626>. Comprehensive instructions will guide you step-by-step on how to fill out and submit the application form. Kindly send all file attachments in Word or Acrobat format. For further details refer to [www.iiserpune.ac.in/~smr2626](http://www.iiserpune.ac.in/~smr2626).

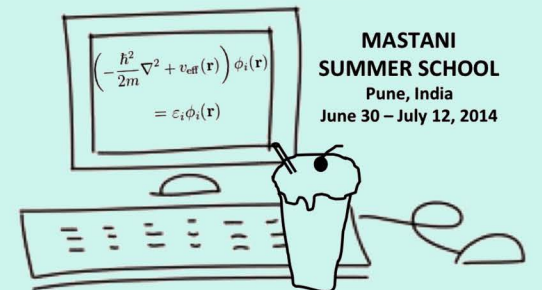
Secretariat: Ms. Rosa del Rio (smr 2626)

Telephone: +39-040-2240396 - Telefax: +39-040-22407396 - E-mail: [smr2626@ictp.it](mailto:smr2626@ictp.it),

[smr2626@iiserpune.ac.in](mailto:smr2626@iiserpune.ac.in)

ICTP Home Page: <http://www.ictp.it>

January 2014



MASTANI  
SUMMER SCHOOL  
Pune, India  
June 30 – July 12, 2014

### Organizers

Prasenjit Ghosh  
(IISER Pune, India)

Shobhana Narasimhan  
(JNCASR, Bangalore, India)

Stefano de Gironcoli  
(SISSA, Trieste, Italy)

Ralph Gebauer  
(ICTP, Trieste, Italy)

### Local Organizer in India

Mukul Kabir  
(IISER Pune, India)

### List of Speakers

P. S. Anilkumar, IISc, Bangalore (India)  
Stefano Baroni, SISSA, Trieste (Italy)  
Cyrille Barreateau, CEA Saclay (France)  
Matteo Cococcioni, EPFL Lausanne (Switzerland)  
Indra Dasgupta, IACSS, Kolkata (India)  
\*Tanusri Saha Dasgupta, SNBNCBS, Kolkata (India)  
Stefano de Gironcoli, SISSA, Trieste (Italy)  
Ralph Gebauer, ICTP, Trieste (Italy)  
Ivan Girotto, ICTP, Trieste (Italy)  
Manish Jain, IISc, Bangalore (India)  
Dilip G. Kanhere, Univ. of Pune, Pune (India)  
\*G. V. Pavan Kumar, IISER, Pune (India)  
Margherita Marsili, Univ. of Padova (Italy)  
Sunil Nair, IISER, Pune (India)  
Shobhana Narasimhan, JNCASR, Bangalore (India)  
Sandro Scandolo, ICTP, Trieste (Italy)  
Ari Seitsonen, University of Zurich, (Switzerland)  
Prasenjit Sen, HRI, Allahabad (India)  
David Vanderbilt, Rutgers University (USA)  
Umesh V. Waghmare, JNCASR, Bangalore (India)

\*To be confirmed

# DEADLINE

## March 31, 2014