



The Abdus Salam

International Centre  
for Theoretical Physics

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IAEA  
International Atomic Energy Agency

## **School on Numerical Methods for Materials Science Related to Renewable Energy Applications**

**26 – 30 November 2012**

**(Miramare - Trieste, Italy)**

The Abdus Salam International Centre for Theoretical Physics is organizing a *School on Numerical Methods for Materials Science Related to Renewable Energy Applications* to be held at ICTP, Trieste, Italy from 26 to 30 November 2012.

*The aim of this school is to teach students and young postdocs the use of state-of-the-art numerical techniques in the broad area of atomistic materials science. In theoretical lectures the employed numerical theories will be explained, while in hands-on computer sessions those approaches will be applied in test systems. The theoretical lectures will be complemented by experimental talks which illustrate concrete research projects. The school will focus on such methods which are of particular importance in the growing area of materials for energy applications.*

The topics of the school will include:

- ✦ Classical molecular dynamics
- ✦ First principles molecular dynamics (Car-Parrinello)
- ✦ Improved sampling methods, metadynamics
- ✦ Computational core level spectroscopy
- ✦ Electronic excitations / quasiparticles from TDDFT and many-body perturbation theory (GW approximation)

### **Participation**

Applicants from all countries that are members of the United Nations, UNESCO or IAEA may attend. As the School will be conducted in English, participants should have an adequate working knowledge of this language. Although the main purpose of the Centre is to help research workers from developing countries through a programme of training activities within a framework of international cooperation, a limited number of students and post-doctoral scientists from developed countries are also welcome to attend.

**Only students and postdocs with proven experience in atomistic computer simulations are eligible for participation in this school.**

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, and who are not more than 45 years old. Such support is available only to those attending the entire activity. *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?2376>. 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.

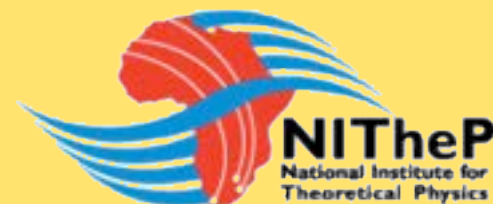
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ICTP Home Page: <http://www.ictp.it>

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**Co-sponsored by:**  
**South Africa's National Institute  
for Theoretical Physics (NITheP)**



### **Organizers**

**Filippo De Angelis**  
(CNR, Perugia, Italy)

**Stefano Fabris**  
(CNR-IOM and  
SISSA, Trieste, Italy)

**Ralph Gebauer**  
(ICTP, Trieste, Italy)

**Nicola Seriani**  
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## **DEADLINE**

**26 August 2012**  
**(if requesting funds  
and/or visa assistance)**

**30 September 2012**  
**(otherwise)**