The Abdus Salam
International Centre for Theoretical Physics

15th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

13 - 15 January 2011

(Miramare - Trieste, Italy)

This Workshop will follow the series started in Oxford, U.K. (1983) and continued in Braunschweig, Germany (1984) and in Trieste, Italy (1987, 1989, 1991, 1993, 1995, 1997, 1999, 2001, 2003, 2005, 2007 and 2009). Following the tradition of the previous meetings, the Workshop will be devoted to recent advances in computational condensed matter physics and materials science, based on realistic calculations of the electronic structure of complex systems.

The activity will be held at the Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy from 13 to 15 January 2011 with the co-sponsorship of the International School for Advanced Studies (SISSA) and the CNR-IOM DEMOCRITOS Simulation Center.

As in previous events of this series, the Workshop will consist of invited talks and a contributed poster session, with ample space devoted to discussion.

Theory and Methods:
Density-Functional Theory beyond LDA
Time Dependent DFT
Many-Body Techniques for Real Materials
Quantum Monte Carlo
Ab-initio Molecular Dynamics
Large-Scale and Multiscale Simulations
Activated Processes
Electronic Transport
Response to External Fields
Simulations in Realistic Environments

Applications:
Nanoscience
Biochemistry and Biomaterials
Magnetism and Spintronics
Geophysics
Functional Materials
Surfaces
Spectroscopies
Catalysis and Electrochemistry
Chemical Reactions and Kinetics
Materials Design

PARTICIPATION: Scientists from all countries that are members of the United Nations, UNESCO or IAEA may attend the Workshop. As the activity will be conducted in English, participants should have an adequate working knowledge of this language. There is no registration fee. Travel and subsistence expenses of participants should be borne by their home institutions. Limited funds are available for some participants who are nationals of, and working in, a developing country, to be selected by the Organizers. However, every effort should be made by candidates to secure at least partial support for their travel expenses.

CALL FOR CONTRIBUTED POSTERS: During the activity there will be a Poster Session. Abstracts must be submitted to the Workshop Secretary, at the address indicated below. The recommended format for the abstracts (including title, authors and abridged institutions) is 16 cm (wide) by 11 cm (high). Please send file attachments in PDF format by **1 November 2010**.

Hands-on tutorial on Electronic Structure Computations

A **Hands-on Tutorial on Electronic Structure Computations** will be organized in the week following the Workshop, January 17-21, 2011. Advanced topics like electronic transport, excitations (TDDFT and GW) and NRM computations will be treated. Students and young postdocs with a proven experience in standard DFT computations may participate in this tutorial. The Tutorial is open only for participants of the Workshop.

HOW TO APPLY: The online application form can be accessed on the activity's website:
http://agenda.ictp.it/smr.php?2220
Once in the website, comprehensive instructions will guide you step-by-step on how to fill out and submit the application form. This application form is also valid for the Hands-on Tutorial.

SECRETARIAT

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

Trieste, August 2010

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D. Vanderbilt
(Rutgers University, New Brunswick, USA)

Deadlines:

22 September 2010
(if requesting funds)

and

1 November 2010
(if NOT requesting funds)