



The Abdus Salam
International Centre for Theoretical Physics


United Nations
Educational, Scientific
and Cultural Organization


International Atomic
Energy Agency

**13th International Workshop on
Computational Physics and Materials Science:
Total Energy and Force Methods**

11 - 13 January 2007
(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 and 2005). 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 11 to 13 January 2007 with the co-sponsorship of the International School for Advanced Studies (SISSA) and the INFN DEMOCRITOS National Simulation Center.

As in previous events of this series, the Workshop will consist of invited talks 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

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 deadline for receipt of the contributed papers is **1 December 2006**. 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.

PARTICIPATION: Scientists from all countries which 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. As a rule, travel and subsistence expenses of participants should be borne by the home institution. 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, to be selected by the Organizers. There is no registration fee to attend this activity.

The Application Form is obtainable from the Activity Web page:
<http://agenda.ictp.it/smr.php?1824> (which will be constantly up-dated)
or from the Activity Secretariat: (smr1824@ictp.it)

The form should be completed, signed and returned to:
the Abdus Salam International Centre for Theoretical Physics
smr1824
(c/o Ms. Doreen Sauleek),
Strada Costiera 11, I-34014 Trieste, Italy

or send via email to: smr1824@ictp.it
(please save and send file attachments in PDF format)

or send via telefax to no: +39 040 224163

Telephone: +39-040-2240346

Telefax: +39-040-224163

E-mail: smr1824@ictp.it

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

(also reachable through: <http://www.democritos.it/events/totalenergy-XIII/totalenergy-XIII.php>)

Trieste, August 2006

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(Rutgers State University, Piscataway, USA)

Deadlines:

1 October 2006
(if requesting funds)

or

1 November 2006
(if NOT requesting funds)