

TWELFTH INTERNATIONAL WORKSHOP on COMPUTATIONAL PHYSICS AND MATERIALS SCIENCE: TOTAL ENERGY AND FORCE METHODS

13 - 15 January 2005
Miramare - Trieste, Italy

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

The activity will be held at the Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy, from 13 to 15 January 2005 with the **co-sponsorship of the International School for Advanced Studies (SISSA) and of 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.

TOPICS COVERED INCLUDE:

- Density-functional molecular dynamics
- Large-scale electronic structure calculations
- Linear-scaling methods
- Density-functional theory beyond the local-density approximation
- Quantum Monte Carlo
- Many-body techniques for real materials
- Multiple time and length scales in computer simulations
- Relativistic effects in electronic structure
- Computer-science tools
- Applications to:
 - Transition states and rates
 - Non-equilibrium and non-adiabatic processes
 - Electron dynamics and excited states (optical properties)
 - Electric polarization, fields and currents
 - Surfaces and other low-dimensional systems
 - Phase transitions
 - New materials
 - Catalysis
 - Core levels
 - Geophysics
 - Liquids
 - Magnetism and spintronics
 - Nanoscience (nanotribology, transport in nanostructures)
 - Biomolecular materials

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 contributed papers is 3 December 2004. 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 or RTF formats.

PARTICIPATION

Scientists from all countries that are members of the UN, UNESCO or IAEA may attend the Workshop. As the activity will be conducted in English, participants should have an adequate working knowledge of that language. As a rule, travel and subsistence expenses for the participants are borne by their home institutions. However, limited funds are available for some applicants who are nationals of, and working in, developing countries, to be selected by the organizers. As scarcity of funds allows travel to be granted only in a few exceptional cases, every effort should be made by candidates to secure support for their fare (or at least half-fare) from their home country. There is no registration fee to attend this activity.

The Request for Participation Forms can be downloaded, through the ICTP WWW Server, from the activity's WEB Page (<http://agenda.ictp.trieste.it/smr.php?1641>), which will be constantly updated.

The closing dates for the RECEIPT of requests for participation are:

- **15 October 2004** (if requesting financial support and/or requiring visa - please use Form A)
- **15 November 2004** (if neither requesting financial support nor requiring visa; late requests may still be considered if received before 3 December 2004 - please use Form B)

The forms should be completed, signed and returned to:

SMR.1641 c/o Ms. N. Ivanissevich
the Abdus Salam ICTP
Strada Costiera, 11
I-34014 Trieste, Italy

telefax to:
or +39-040-224163 or

e-mail to:
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(please send file attachments
only in RTF or PDF formats)

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M. Parrinello, ETHZ & CSCS, Zürich, Switzerland
D. Vanderbilt, Rutgers University, Piscataway, USA

DEADLINES:

15 October 2004
(IF REQUESTING FUNDS)

or

15 November 2004
(IF NOT REQUESTING FUNDS)

WORKSHOP WEB PAGES:

<http://agenda.ictp.trieste.it/smr.php?1641>

also reachable through:

[http://www.democritos.it/events/
totalenergy-XII/totalenergy-XII.php](http://www.democritos.it/events/totalenergy-XII/totalenergy-XII.php)