

The Abdus Salam International Centre for Theoretical Physics

School on Electronic Structure Methods

14 - 25 July 2008

Cape Town, South Africa

Venue: AIMS, Cape Town, South Africa

The Abdus Salam International Centre for Theoretical Physics, in collaboration with the National Institute for Theoretical Physics, the INFM-DEMOCRITOS National Simulation Center and the International Center for Materials Research, are organizing a School on Electronic Structure Methods from 14th July to 25th July, 2008 in Cape Town, South Africa.

The School will cover the fundamentals of modern electronic-structure theory based on density functional theory, with emphasis on the pseudopotential/plane-wave approach, together with some of the most relevant recent developments and applications.

The activity will be divided into three parts:

- a) a basic introduction to computational materials theory, with an emphasis on density functional methods
- b) a two-day advanced session, highlighting recent developments and applications of electronic structure methods in materials science, nanoscience, surface science, etc.
 c) hands-on computer sessions based on the "quantum-espresso" distribution of codes for plane-wave pseudopotential calculations



CO-SPONSORS

The Abdus Salam International Centre for Theoretical Physics (ICTP) Trieste, Italy

ΙΑΕΑ

National Institute for Theoretical Physics (NITheP), South Africa

INFM-DEMOCRITOS National Simulation Center, Trieste, Italy

International Center for Materials Research (ICMR), Santa Barbara, USA

A "Pre-School" will be held to enable a broader group of participants to access the School by providing background in condensed matter physics and computational methods. The preschool will be held July 7-11 in conjunction with the meeting of the South African Institute of Physics in Polokwane, South Africa. Limited funds are available to help cover costs for participants. Information and application forms are available at <u>http://neo.phys.wits.ac.za/school/</u>.

PARTICIPATION

Scientists and students from all countries which are members of the United Nations, UNESCO or IAEA may attend the School. Given the regional character of the initiative, applications from African countries will be privileged. The school will be conducted in English. Participants are required to have a basic knowledge of Linux. As a rule, travel and subsistence expenses of the 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, and who are not more than 45 years old. There is no registration fee.

The Application Form is obtainable from the ICTP website:

<u>http://agenda.ictp.it/smr.php?1979</u> or from the Activity Secretariats (addresses below). It should be completed and returned by e-mail (as file attachment: either PDF, RTF or .doc) before <u>31 March 2008</u> as follows:

For applicants from South Africa: to Professor Daniel Joubert, School of Physics, University of the Witwatersrand, Private Bag X3, Wits 2050, South Africa - e-mail: Daniel.Joubert@physics.org

For applicants from all other regions and countries:

to the Abdus Salam I.C.T.P. (Ref: smr 1979) - Strada Costiera, 11 - 34014 Trieste, Italy (e-mail: smr1979@ictp.it, fax +39-040-2240354)

Centre for High Performance Computing (CHPC), Cape Town, South Africa

Materials Computation Center (MCC), Urbana, IL, USA

DIRECTORS

Richard MARTIN (USA) Hafid AOURAG (Algeria) Paolo GIANNOZZI (Italy) Daniel JOUBERT (South Africa) Sandro SCANDOLO (Italy)

LECTURERS

Visit http://neo.phys.wits.ac.za/school/ for updates

DEADLINE for requesting participation

31 MARCH 2008

For enquiries please contact: Daniel.Joubert@physics.org or smr1979@ictp.it