ICTP - INFM-DEMOCRITOS - ISMO - IUT School on: Electronic-structure calculations and their applications in materials science

25 April - 6 May 2005

Isfahan, Iran

A School on: Electronic-structure calculations and their applications in materials science will be held at the Isfahan University of Technology (IUT) in Iran from 25 April to 6 May 2005. The School will be jointly sponsored by the Abdus Salam International Center for Theoretical Physics (ICTP, http://www.ictp.trieste.it), the Italian INFM-DEMOCRITOS National Simulation Center (http://www.democritos.it), the Center for International Research & Collaboration (ISMO, http://www.ismo.ir), and organized in collaboration with the Isfahan University of Technology (IUT, http://www.iut.ac.ir). The directors are: Hadi Akbarzadeh (IUT), local organizer, Stefano Baroni (Scuola Internazionale Superiore di Studi Avanzati-SISSA and DEMOCRITOS, Trieste, Italy), Maria Peressi (Università di Trieste and DEMOCRITOS, Trieste, Italy), and Abdallah Qteish (Yarmouk University, Irbid, Jordan).

The School will cover the fundamentals of modern electronic-structure theory based on density functional theory, with strong emphasis on the pseudopotential/planewave approach, together with some of the most relevant recent developments and applications. The School will consist of a three-day international workshop devoted to some of the recent advances in the field, followed by a full-immersion one-week hands-on tutorial course on the use of the PWscf/ESPRESSO suite of computer codes (http://www.pwscf.org, http://www.democritos.it/scientific.php).

A tentative list of speakers and lecturers includes:

Hadi Akbarzadeh (Isfahan University of Technology, Isfahan - Iran) Alfonso Baldereschi (Ecole Polytechnique Fédérale de Lausanne, Switzerland and Università degli Studi di Trieste, Trieste - Italy)**

Stefano Baroni (SISSA, Trieste - Italy)**

Keyvan Esfarjani (Sharif University of Technology, Tehran - Iran)

Stefano de Gironcoli (SISSA, Trieste - Italy)**

Paolo Giannozzi (Scuola Normale Superiore, Pisa - Italy)**

Oguz Gulseren (Bilkent University, Ankara - Turkey)

Volker Heine (Cambridge University, Cambridge – UK)

Nicola Marzari (Massachussetts Institute of Techology, Cambridge - USA)

Noureddine Meskini (Université de Tunis, Tunis - Tunisia)

Maria Peressi (Università degli Studi di Trieste, Trieste - Italy)**

Abdallah Qteish (Yarmouk University, Irbid - Jordan)

Lucia Reining (Ecole Polytechnique, Palaiseau - France)

Carlo Sbraccia * (International School for Advanced Studies, Trieste - Italy)**

Sandro Scandolo (ICTP, Trieste - Italy)**

Nacir Tit (United Arab Emirates University, Al-Ain – United Arab Emirates)

Erio Tosatti (SISSA and ICTP, Trieste - Italy)**

Renata Wentzcovitch (University of Minnesota, Minneapolis - USA)

<u>PARTICIPATION</u>

Scientists and students from all countries which are members of the United Nations, UNESCO or IAEA may attend the School. As it will be conducted in English, participants should have an adequate working knowledge of this language. All participants are also required to have an adequate working knowledge of Linux and Fortran 77/90.

Although the main purpose of the School is to help research workers from developing countries, through a programme of training within a framework of international cooperation, a limited number of students and post-doctoral scientists from developed countries are also welcome to attend.

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. Such support is available only for those who attend the entire duration of the School. There is no registration fee.

The Application Form is obtainable from the ICTP WWW server:

http://agenda.ictp.trieste.it/agenda/current/fullAgenda.php?email=0&ida=a04223 (which will be constantly up-dated) or from the activity Secretariats (address below). It should be completed and a hard copy returned (no applications via e-mail will be considered) before 15 December 2004 as follows:

For applicants from Iran: to Mrs. Shams, International & Scientific Cooperation Office (ISCO), Isfahan University of Technology, Electronic Structure School (Ref. smr.1690), 84154 Isfahan, Iran (phone: +98- 311-3912505 or 2506; fax: +98-311-3912511 e-mail: isco@cc.iut.ac.ir)

For applicants from all other countries: to The Abdus Salam I.C.T.P. - Electronic Structure School in Iran (Ref. smr. 1690)- Strada Costiera, 11 - 34014 Trieste, Italy

(phone: +39-040-2240540 - fax: +39-040-224163 - e-mail: cm@ictp.trieste.it)

CO-SPONSORED BY:

- INFM-DEMOCRITOS National
 - Simulation Center
- Center for International Research & Collaboration (ISMO)

ORGANIZED IN COLLABORATION WITH

Isfahan University of Technology

DIRECTORS

- **H. Akbarzadeh** (IUT), local organizer
- S. Baroni (SISSA & DEMOCRITOS)
- M. Peressi (Università di Trieste & DEMOCRITOS)
- **A. Qteish** (Yarmouk University)

DEADLINE for requesting participation

15 December 2004