The Abdus Salam
International Centre for Theoretical Physics
www.ictp.it

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

SISSA — ma per seguir virtute e canoscenza

DEMOCRITOS DEmocritos MOdeling Center for Research In aTOmistic Simulation — CNR-IOM

ICSU International Council for Science

Hands-on Tutorial on Electronic Structure Computations

14-18 January 2013

(Miramare - Trieste, Italy)

This Hands-on Tutorial will directly follow the "16th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods" (January 10-12, 2013). The goal of this Tutorial is to link the theoretical presentations of the Workshop with practical courses in the ICTP's computer laboratories.

The activity will be held at the Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy from 14-18 January 2013 with the co-sponsorship of CNR-IOM DEMOCRITOS National Simulation Center and SISSA.

The first part of the Tutorial (three days) will focus on key computational techniques employing density-functional theory in a planewave-pseudopotential framework, and will be based on the Quantum ESPRESSO suite of programs. Advanced topics covered will include:

- **electronic transport**
- **excitations (TDDFT and GW)**

The second part of the Tutorial (two days) will be devoted to Quantum Monte Carlo (QMC). The main focus will be on:

- **variational and diffusion QMC**

the most widely used techniques for electronic structure calculations. The QMC tutorial will include hands-on sessions for total-energy computations of condensed systems.

Given the advanced level of the topics, students and young post-docs with a proven experience in *ab initio* electronic structure computations may apply to participate in this Tutorial. Please note that the Tutorial is open only for participants of the Workshop.

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 the home institution. 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.

HOW TO APPLY: Application for this Tutorial is only possible in conjunction with the application for the "16th International Workshop on Computational Physics and Materials Science". The online application form for both activities can be accessed on the activity's website:. http://cdsagenda5.ictp.it/full_display.php?ida=a12255

Once in the website, comprehensive instructions will guide you step-by-step on how to fill out and submit the application form by 24 September 2012 if you are requesting funding, or by 5 November 2012 if you do not require financial assistance.
NB/ Applications to attend the Tutorial only will not be considered.

SECRETARIAT:

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Directors

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SISSA & DEMOCRITOS,
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Deadlines:

24 September 2012
(if requesting funding)

5 November 2012
(if not requesting funding)

Trieste, November 2012