

Hands-on Tutorial on Electronic Structure Computations

17-21 January 2011

(Miramare - Trieste, Italy)

This Hands-on Tutorial will directly follow the "15th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods" (January 13-15 2011) . The goal of this Tutorial is to link the theoretical presentations of the Workshop with hands-on exercises in ICTP's computer laboratories.

The activity will be held at the Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy from 17-21 January 2011 with the co-sponsorship of INFM DEMOCRITOS National Simulation Center and SISSA.

The Tutorial, based on the Quantum ESPRESSO suite of programs, will focus on advanced computational techniques employing density-functional theory in a planewave-pseudopotential framework. The covered themes include

- electronic transport,
- excitations (TDDFT and GW)
- NMR computations.

Because of the advanced nature of these topics, prior experience and knowledge of basic ground-state DFT computations is indispensable for participation in the Tutorial.

Students and young post-docs <u>with a proven experience in standard DFT</u> <u>computations</u> 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.

Directors

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HOW TO APPLY

Application for this Tutorial is only possible in conjunction with the application for the "15th International Workshop on Computational Physics and Materials Science".

The online application form for both activities can be accessed on the activity's website:. <u>http://agenda.ictp.it/smr.php?2221</u>

Once in the website, comprehensive instructions will guide you step-by-step on how to fill out and submit the application form by 22 September 2010 if you are requesting funding, or by 1 November 2010 if you do not require financial assistance.

NB/ Applications to attend the Tutorial only will not be considered.

SECRETARIAT

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Trieste, August 2010



22 September 2010 (if requesting funding)

<u>**1 November 2010**</u> (if not requesting funding)