



Advanced Workshop on High-Performance & High-Throughput Materials Simulations using QUANTUM ESPRESSO

from 16 to 27 January, 2017

The Abdus Salam International Centre for Theoretical Physics, in collaboration with the Quantum ESPRESSO Foundation and the MaX EU Centre of Excellence for HPC applications, with the participation of CECAM, the Psi-k electronic-structure network, the MARVEL National Centre of Competence in Research and the eCam EU Centre of Excellence for HPC applications, is organizing a two-week Workshop in advanced techniques for large-scale quantum materials modeling.

The goal of the Workshop is to enable participating scientists to combine the most advanced approaches to quantum materials simulation with an in-depth understanding of modern parallel architectures. The intensive program will offer theoretical and technical lectures, as well as demonstrations and dedicated hands-on sessions exploring the most relevant HPC resources for scientific production. Participants will learn how to handle the research codes in the QUANTUM ESPRESSO more efficiently, and to handle the AiiDA framework to manage, store, share, and disseminate the workload. Hands-on sessions will be held on the SISSA-ICTP facility for high-end computing.

GRANTS

Thanks to generous support from a number of sponsors and funders, fellowships are available for the highest-ranked candidates. The fellowships include partial support for accommodation at an ICTP Guest House. Fellowships are granted only if attending at the entire two-weeks programm.

In addition, a limited number of grants are available to support the travel, lodging and living expenses of selected participants, with priority given to those working in a developing country who are at the early stages of their career. Financial support to participants from developed countries is provided only if specifically requested within the final "comments" session of the application form and supported with a recommendation letter.

Free meal coupons for the ICTP cafeteria will be provided to all participants.

INDUSTRIAL PARTICIPATION

Industrial participation is strongly encouraged, either from researchers active in materials modelling or in scientific software development. No registration fees required.

HOW TO APPLY FOR PARTICIPATION:

The Online Application Form can be accessed through the School website along with comprehensive instructions that will guide you step-by-step on how to fill out and submit the Application Form: <http://indico.ictp.it/event/7921/>

The Workshop will be conducted in English. A working knowledge of the Linux environment and of QUANTUM ESPRESSO or comparable electronic-structure codes will be greatly beneficial.

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Directors:

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(University of Udine)

Nicola Marzari (EPFL)

Local Organizers:

Ralph Gebauer (ICTP)

Ivan Girotto (ICTP)

Other Invited Speakers:

Oliviero Andreussi
(USI/EPFL)

Carlo Cavazzoni
(CINECA)

Giovanni Pizzi
(EPFL)

Iurii Timrov
(EPFL)

DEADLINE

"A deadline extension is foreseen
for applications not requiring
VISA"

16 October 2016

