QUANTUM ESPRESSO WORKSHOP 2014
June 16-20, 2014

Penn State University · Cybertorium (113 IST Building) · University Park · PA, USA

Overview

Penn State University, through its Research Computing and Cyberinfrastructure unit and the Materials Simulation Center, announces a Quantum ESPRESSO Workshop.

Quantum Espresso is a modular and open-source suite widely used in the investigation of the properties of man-made and natural materials, taking explicitly into account the electronic structure. Developers of the package, led by the Professors Stefano Baroni and Paolo Giannozzi will present the theory behind the codes and train the participants on how to use them for different applications. Participants would be able to present a poster of their own work during the workshop. Lectures, tutorials and poster sessions will be held from 8:00AM to 6:00PM, including twenty m**inutes** coffee breaks and two hours for lunch.

Questions, comments, and suggestions are welcome!

Confirmed Lecturers

Stefano Baroni • SISSA and CNR-IOM DEMOCRITOS, Italy
Paolo Giannozzi • University Udine and CNR-IOM DEMOCRITOS, Italy
Marco Buongiorno Nardelli • University of North Texas, USA
Marco Fornari • Central Michigan University, USA
Burak Himmetoglu • University of California, Santa Barbara, USA
Nicolas Poilvert • Penn State University, USA

Organizers

Lazaro Calderin • Penn State University, USA • calderin@psu.edu
Ismaila Dabo • Penn State University, USA • dabo@psu.edu

Registration

The registration fee for the workshop is $675.00 and covers the workshop materials, lunch for the five days and the conference dinner. The last date to register will be June 10, 2012. We offer a discount for early registration; if you register before May 29, the registration fee is $600.00.

URL msc.psu.edu/qe2014

Preliminary Program

Day I | Monday, June 16, 2014

Introduction to Density-functional Theory
Introduction to Quantum Espresso
Hands-on: Self-consistent-field Calculations
Hands-on: Structural Optimization

Day II | Tuesday, June 17, 2014

Advanced Functionals: Van der Waals and Hybrids
Advanced Functionals: DFT+U
Hands-on: Van der Waals and Hybrid Funcitonals
Hands-on: DFT+U

Day III | Wednesday Jun 18, 2014

Density-functional Perturbation Theory
Phonons Calculations
Hands-on: Phonons I
Hands-on: Phonons II

Day IV | Thursday Jun 19, 2014

High-throughput Calculations
Hands-on: High-throughput
Transport Properties
Hands-on: Transport properties

Day V | Friday Jun 20, 2014

TD-DFPT (Time-dependent Density-functional perturbation theory)
TD-DFPT Implementation
Hands-on: TD-DFPT I
Hands-on: TD-DFPT II