Quantum-Espresso Workshop

The Pennsylvania State University · University Park, PA · USA

May 21-25, 2018

Overview

The Materials Computation Center of the Materials Research Institute at Pennsylvania State University announces the 2018 Quantum-Espresso Workshop.

Quantum-Espresso is an open-source software widely used for predicting the properties of materials from first principles. In this workshop, developers of the package, led by Dr. Stefano Baroni, will present the theory behind the codes and train the participants on how to use them for different applications, including the calculation of structural, vibrational, optical, and transport properties and the use of high-throughput software capabilities for computational materials screening.

Participants will have the opportunity to present a poster during the workshop.

Speakers

Stefano Baroni · International School for Advanced Studies, SISSA · Italy
Oliviero Andreussi · University of North Texas · USA
Marco Buongiorno Nardelli · University of North Texas · USA
Marco Fornari · Central Michigan University · USA
Roxana Margine · Binghamton University · USA
Michele Pavanello · Rutgers University · USA

Organizers

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Registration

Registration is now open. The registration fee for the workshop is of $600 if you register before April 30 ($300 for Penn State affiliates) and of $675 after this date. The last date to register is May 14. The registration fee covers workshop materials, lunch for the five days, and the conference dinner.

Funding

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www.mri.psu.edu/mri/events/quantum-espresso

Program

Day 1 | May 21, 2018

Overview of Density-functional Theory
Introduction to Quantum-Espresso

Hands-on: Self-Consistent-Field Calculations
Hands-on: Equilibrium Structure Calculations

Day 2 | May 22, 2018

Density-Functional Perturbation Theory
Hands-on: Phonons

Time-Dependent
Density-Functional Perturbation Theory
Hands-on: Absorption Spectra Calculations

Day 3 | May 23, 2018

High Throughput and Data Mining
Hands-on: Automated Calculations (AFLOWπ)

Transport and Optical Properties
Advanced Functionals
Hands-on: Automated Calculations (PAOFLOW)

Day 4 | May 24, 2018

Implicit Solvation
Hands-on: Quantum-Continuum Calculations

Quantum Embedding
Hands-on: Frozen Density Embedding Models

Day 5 | May 25, 2018

Electron-Phonon Interactions
Hands-on: Electron-Phonon Calculations