Interdepartmental Doctoral Degree Program for Multi-dimensional Materials Science Leaders

First Principles Workshop

An introduction and hands-on tutorial with the Quantum ESPRESSO

Friday, February 26, 2016 @ Department of Physics, Tohoku University

Today's most popular method for calculating the electronic structures of atoms, molecules, and solids is based on first principles density functional theory (DFT) calculation. This method is based on the solution of the Schrödinger equation for the electrons, without any empirical inputs, and thus it allows us for accurately describing the mechanical, physical, and chemical properties of materials. Quantum ESPRESSO (QE) is currently recognized to be one of the most widely used packages for the DFT calculations, and it has been under continuous development since many years, thanks to its open-source and great community support.

The aim of this workshop is to bring together graduate students and young scientists working with QE, as well as general people with interest in QE. The workshop will cover basic concepts and recent advances and developments of QE, including geometry optimizations, band structure, linear-response theory and phonons, transport, and thermoelectric power of some materials, including graphene and carbon nanotubes.

What we will learn in Workshop

Quantum ESPRESSO (QE)
Structural Optimization, Electron Structures, Phonon Dispersions.
http://www.quantum-espresso.org/

Wannier90
Quantum Transport, Thermoelectric.
http://www.wannier.org/

Yambo
Spectroscopy, Electronic Excitations.
http://www.yambo-code.org/

Big Data
Database of **1,045,803** material compounds (including data file for QE).
http://aflowlib.org/

For Participants: We will lend you a USB 32G including Linux live, QE, Wannier90, Yambo packages, lectures and related materials. However, you should bring your laptop. If you do not have a laptop, please contact us for assistance. All the participants are kindly requested to make the registration of the workshop before **Feb. 20, 2016** by accessing**:**
https://sites.google.com/site/fpw2016md/
The workshop is totally free.

Sponsor
Interdepartmental Doctoral Degree Program for Multi-dimensional Materials Science Leaders
Web: http://m-dimension.tohoku.ac.jp/

Organizing Committee
N. T. Hung
A. R. T. Nugraha

Lectures
Prof. Riichiro Saito
Dr. A. R. T. Nugraha
N. T. Hung
P. Ayria
Y. Tatsumi

Location
Room 721, H-03 (Science Complex B), Tohoku University Aobayama Campus

Date & Time
Friday, February 26, 2016
9:30 a.m. to 3:00 p.m.

Contact us
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