Computer modelling of materials at the nanoscale

An introduction and hands-on tutorial with the
QUANTUM ESPRESSO & YAMBO codes

The Department of Chemical System Engineering of the University of Tokyo

(www.tcl.t.u-tokyo.ac.jp),

in collaboration with the Quantum ESPRESSO Foundation

(http://foundation.quantum-espresso.org)

organises a four-day training course to be held at the

Sanjo Conference Hall,

The University of Tokyo, Hongo campus, 23-26th April, 2014.

Starting from a general revise of the DFT capabilities for electronic structure calculation and geometry optimization of periodic and finite systems, emphasis will be set during the course to the dynamical processes and excited-state properties dealt by means of both Time Dependent DFT and Many Body Perturbation Theory.

- Day 1 (Apr 23rd): Morning - A DFT primer with applications to the electronic structure, structural stability, and geometry optimisation of finite and periodic systems.
  Afternoon: hands-on tutorial with the QUANTUM ESPRESSO distribution.

- Day 2 (Apr 24th): Simulation of rare events, location of transition states, evaluation of energy barriers. (NEB, metadynamics, basin hopping).
  Afternoon - hands-on tutorial with the QUANTUM ESPRESSO distribution.

- Day 3 (Apr 25th): DFT-based simulation of excited-state properties. DFPT for lattice and molecular vibrations, TDDF(p)T for optical excitations electron-energy loss spectroscopies.
  Afternoon - hands-on tutorial with the QUANTUM ESPRESSO distribution.

- Day 4 (Apr 26th): Simulation of excited-state properties from many-body perturbation theory.
  Afternoon - hands-on tutorial with the YAMBO code

List Of Speakers (in alphabetic order)

Prof. Stefano Baroni (SISSA, Italy); Dr. Stefano Fabris (CNR-Democritos, Italy); Prof. Paolo Giannozzi(University of Udine, Italy); Dr. Andrea Marini (CNR, Italy); Dr. Yoshitaka Tateyama(NIMS, Japan).

Format
Morning (9am-12pm) frontal lectures
Afternoon (2pm-5pm) computer lab

The following prerequisites are requested to the participants:

Acquaintance with basic electronic-structure theory, based on density-functional theory, rudiments of many-body perturbation theory will be a plus; Elementary working experience with the UNIX operating system; Possession of a laptop that each participant will use to access the HPC resources used for the hands-sessions. Minimum hardware/software requirements include a wifi card and a working X11 windowing system; Proficiency in English language.

Tutorial fee: 50.000 JPY (Company employees); 20.000 JPY (Academic Staff); 8.000 JPY (PhD, MA, BA Students).

Local Organizing Committee:

Academic: Prof. Koichi Yamashita, Dr. Giacomo Giorgi, Dr. Mikiya Fujii, Dr. Ryota Jono, Mr. Hiroki Kawai, Ms. Ayako Kubo.
Secretary: Mrs. Mayumi Iyama

For further information & applications please contact Dr. Giorgi
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(replace "_at_" with "@")