

Computer modelling of materials at the nanoscale

*An introduction and hands-on tutorial with the
QUANTUM ESPRESSO distribution & YAMBO code*

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 introduction to DFT for electronic-structure calculations and geometry optimization in periodic and finite systems, more advanced topics will be covered, including the simulation of chemical reactivity, using NEB and advanced sampling techniques, and of dynamical processes and excited-state properties using Time Dependent DFT and Many Body Perturbation Theory methodologies.



Lectures will be held by:

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), Dr. Iurii Timrov (SISSA, Italy).

Format of the course: theory lectures in the morning (8.45am-12pm) & hands-on tutorials with the QUANTUM ESPRESSO distribution and YAMBO code in the afternoon (2-6pm)

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: 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 (giacomo_at_tcl.t.u-tokyo.ac.jp)
(replace “_at_” with “@”)