Nov. 24 (Thu) 9:30 - Nov. 25 (Fri) 12:30 (E6, Rm. 5318)

The 2nd OpenMX developer's meeting

The 2nd OpenMX developer's meeting will be held in KAIST, Daejeon, South Korea, for Nov. 24th and 25th, 2016. Recent development and implementation of new functionalities will be discussed including some advanced applications using OpenMX. The meeting will provide a good opportunity for active developers to exchange their ideas, and promote further development of OpenMX. We also encourage researchers, who are interested in contributing to development of OpenMX, to attend the informal meeting.

Nov. 24 (Thu) 9:30 - 17:30, E6 Rm. 5318

Speaker	Topic
T. Ozaki (Univ. of Tokyo)	Core level bindng energies in solids from first-principles
C.-C. Lee (Univ. of Tokyo)	Combining LCAO basis functions with plane waves in OpenMX codes for excitation calculations
Y.-T. Lee (KAIST)	Implementation of phonon dispersion with LO-TO splitting for polar materials
M. J. Han (KAIST)	Calculating branching ratio and spin-orbit coupling from first-principles
M. Shin (KAIST)	DFT-based NEGF simulations of nanoscale FETs
M. Ohfuchi (Fujitsu Lab)	Large-scale electronic structure calculation method in OpenMX
M. Kawamura (Univ. of Tokyo)	Currentdensity and eigenchannel: Implementation and application
M. Fukuda (Univ. of Tokyo)	Toward on O(N) method for the non-equillibrium Green's function calculation
J. Yu (SNU)	Development of OpenMX calculator interface for ASE (Atomic Simulation Environment) and its applications.
T. Ozaki (Univ. of Tokyo)	Development of OpenMX viewer

Nov. 25 (Fri) 9:30 - 12:30, E6 Rm. 5318

Speaker	Topic
H. Weng (CAS)	TBA
H. Sawahata (Kanazawa Univ.)	Z2 topological invariants and Chern number
F. Ishii (Kanazawa Univ.)	Application of interface to Wannier90: anomalous Nernst effect
A. Ito (NIFS)	Hybrid simulations for plasma material interaction with OpenMX
T. Ozaki (Univ. of Tokyo)	Stress and variable cell optimization in OpenMX

Information

Hompage : http://www.openmx-square.org/workshop/meeting16/

Location : Natural Science Building (E6), KAIST, Daejeon, South Korea