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**

T. Ozaki (Univ. of Tokyo)  
C.-C. Lee (Univ. of Tokyo)  
Y.-T. Lee (KAIST)  
M. J. Han (KAIST)  
M. Shin (KAIST)  
M. Ohfuchi (Fujitsu Lab)  
M. Kawamura (Univ. of Tokyo)  
M. Fukuda (Univ. of Tokyo)  
J. Yu (SNU)  
T. Ozaki (Univ. of Tokyo)

**Topic**

Core level binding energies in solids from first-principles  
Combining LCAO basis functions with plane waves in OpenMX codes for excitation calculations  
Implementation of phonon dispersion with LO-TO splitting for polar materials  
Calculating branching ratio and spin-orbit coupling from first-principles  
DFT-based NEGF simulations of nanoscale FETs  
Large-scale electronic structure calculation method in OpenMX  
Current density and eigenchannel: Implementation and application  
Toward on O(N) method for the non-equilibrium Green’s function calculation  
Development of OpenMX calculator interface for ASE (Atomic Simulation Environment) and its applications.

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

**Speaker**

H. Weng (CAS)  
H. Sawahata (Kanazawa Univ.)  
F. Ishii (Kanazawa Univ.)  
A. Ito (NIFS)  
T. Ozaki (Univ. of Tokyo)

**Topic**

TBA  
Z2 topological invariants and Chern number  
Application of interface to Wannier90: anomalous Nernst effect  
Hybrid simulations for plasma material interaction with OpenMX  
Stress and variable cell optimization in OpenMX

**Information**

Homepage: http://www.openmx-square.org/workshop/meeting16/  
Location: Natural Science Building (E6), KAIST, Daejeon, South Korea