

Nov. 23 (Wed) 13:30 - 17:30 (E6, Room 1323)

# Hands-on workshop of OpenMX



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.

Before the two day meeting, we will organize a hands-on workshop of OpenMX in KAIST on 23rd. Students and researchers, who are interested in density funtional theories (DFT) calculations, and using OpenMX, are expected to attend the hands-on workshop. We are looking forward to having stimulating discussion in KAIST.

## Hands-on Workshop of OpenMX (Nov. 23 13:30 - 17:30, E6 Rm. 1323)

### Speaker

T. Ozaki (Univ. of Tokyo)

T. Ozaki (Univ. of Tokyo)

H. Weng (CAS)

T. Ozaki (Univ. of Tokyo)

C.-C. Lee (Univ. of Tokyo)

T. Ozaki (Univ. of Tokyo)

### Topic

Overview of DFT

Localized basis methods in OpenMX

Wannier functions in OpenMX

Electronic transport calculation method in OpenMX

Unfolding band structure into a conceptual Brillouine zone

Large-scale electronic structure calculation method in OpenMX

### Information

Homepage : <http://www.openmx-square.org/workshop/meeting16/>

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

