PCoMS & RISME TOMBO Seminar :
First-Principles Theory, Computation, and Hands-On 2022

Overview

This seminar is for anyone, who is interested in the first-principles code, TOMBO. TOMBO uses the all-electron mixed basis approach, in which one-electron orbitals are expressed with both plane waves and atomic orbitals. TOMBO can handle both isolated systems and crystal (or periodic) systems in a unified way. It can perform not only LDA calculations but also GW (+ Bethe-Salpeter equation) calculations. It also handles the TDDFT dynamics simulations in the excited states as well as the usual first-principles molecular dynamics (MD) simulations in the ground state. The hands-on tutorial is about 2 and half hours including (1) GW+Bethe-Salpeter calculation for Li_2, (2) LDA band calculation for Si crystal, (3) first-principles MD simulation for the chemical reaction CO_2 +2H → HCOOH, and (4) GW calculation for Si crystal.

March 23 (WED.), 2022 9:30 ▸17:30
(Lunch break 11:45-13:00)

Registration:

Pre-registration required by 13:00 on Mar. 22
free of charge
http://pcoms.imr.tohoku.ac.jp/R03/PCoMS-TOMBO-2022Mar/

Capacity: 50 persons

Online virtual meeting

Notes:
Hands-on training is done on Windows 10 or newer (64 bit OS) PC.

Lecturers
(listed in presentation order)

Yoshiyuki Kawazoe (NICHe, Tohoku Univ.)
Hiroshi Mizuseki (KIST, Korea)
Kaoru Ohno (Yokohama National Univ.)
Takeshi Nanri (Kyushu Univ.)
Riichi Kuwahara (Dassault Systemes)
Ryoji Sahara (NIMS)

Cohosted by PCoMS http://pcoms.imr.tohoku.ac.jp/
RISME http://risme.imr.tohoku.ac.jp/
Cosponsered by CCMS, IMR, Tohoku Univ. https://www.sc.imr.tohoku.ac.jp/

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Programs

9:30-10:30	**Introduction to First-Principles Calculation** Yoshiyuki Kawazoe (NICHe, Tohoku Univ.)
10:30-11:00	**Application to High Entropy Alloys using VASP** Hiroshi Mizuseki (KIST, Korea)
11:00-11:45	**Theory and Application to Excited States** Kaoru Ohno (Yokohama National Univ.)
11:45-13:00	Lunch break
13:00-13:30	**Results of Performance Tuning on TOMBO** Takeshi Nanri (Kyushu Univ.)
13:30-14:10	**GWΓ + BSE, user interface for TOMBO** Riichi Kuwahara (Dassault Systemes)
14:10-14:50	**GW, TDDFT, how to use TOMBO** Ryoji Sahara (NIMS)
14:50-17:10	**TOMBO Hands-on Tutorial**
17:10-17:30	**Q&A**

<Notes>

*The members of PCoMS IPD program (fellow and general) can earn 1 credit of PCoMS IPD elective course category (A & B), if he or she attends this seminar.

Category A: Wide knowledge of computational materials science

Category B: High-performance computing technologies and techniques