

Mini-workshop on first-principles calculation and its application to computational materials design

Sponsor: Center for Spintronics Research Network (CSRN), Graduate School of Engineering Science.

The University of Osaka, Spintronics Research Network Division, OTRI, The University of Osaka.

Date and Time: 5 June 2025, 10:00~16:30

Place: The University of Osaka, Suita Campus, R4 building 2F meeting room

Program:

Session 1 (10:00 ~ 11:50, Chair: Sato)

10:00~10:30 **Biplab Sanyal** (Uppsala University)

Magnetism and spin transport in 2D magnets and their heterostructures

10:30~10:50 **Kazunori Sato** (GSE, The University of Osaka)

KKR-CPA method and its application to computational design of functional materials

10:50~11:10 **Takao Kotani** (Tottori University)

GPU-accelerated quasiparticle self-consistent GW applied to thousands of materials

11:10~11:30 **Tamio Oguchi** (CSRN, The University of Osaka)

Bias dependence of magnetoresistance in Heusler alloy/Ge devices: Boltzmann theory approach

11:30~11:50 **Hisazumi Akai** (GSE, The University of Osaka)

First-principles calculation of finite temperature magnetic and transport properties

11:50~13:00 Lunch

Session 2 (13:00~14:50, Chair: Katsumoto)

13:00~13:30 **Tran Ba Hung** (AIMR, Tohoku University)

Giant Magnetocaloric Effect in $\text{BiCu}_3\text{Cr}_4\text{O}_{12}$ with Lattice, Electronic, and Magnetic Contributions

13:30~13:50 **Tomoki Yamashita** (Nagaoka University of Technology)

Development of Crystal Structure Prediction Methods and Their Application to the Structural Stability of Transition Metal Oxides

13:50~14:10 **Fumiaki Kuroda** (AIST)

BACCHUS: A surface-structure search program

14:10~14:30 **Koun Shirai** (SANKEN, The University of Osaka)

Problems of first-principles calculations of melting temperature

14:30~14:50 **Dinh Van An** (GSE, The University of Osaka)

An approach for achieving colossal permittivity: polaron dynamics in Nb-doped TiO_2

14:50~15:10 Break

Session 3 (15:10~16:30, Chair: Kotani)

15:10~15:30 **Kunihiko Yamauchi** (CSRN, The University of Osaka)

DFT calculations on altermagnetic materials and their applications

15:30~15:50 **Nguyen Thi Phuong Thảo** (SANKEN, The University of Osaka)

First-Principles Insights into Tunable Magnetism in 2D VI_3 and CrI_3

15:50~16:10 **Hiroshi Katsumoto** (GSE, The University of Osaka)

Spin algebraic formulation of exchange Hamiltonians

16:10~16:30 **Siti Amalia** (GSE, The University of Osaka)

Strain-Driven Control of Electric Polarization & Spin Splitting in the Persistent Spin Helix State of XO_2Y_2 ($\text{X}=\text{W}, \text{Mo}$; $\text{Y}=\text{Cl}, \text{Br}, \text{I}$) Monolayer