

Mini-Workshop on Computational Nanomaterials Science 2018

Date: 27th Nov. 2018

Place: Lecture Room 6, Natural Science and Technology Hall 5, Kanazawa University

Organized by Theoretical and Computational Science Group at Nanomaterials Research Institute (NanoMaRI), Kanazawa University

Co-sponsored by KAKENHI on Innovative Area "Nano-Spin Conversion Science" (17H05180), and "Discrete Geometric Analysis for Materials Design" (18H04481).

9:55 Opening Fumiyuki Ishii

10:00- 10:40 Susumu Minami, "Analysis of Anomalous Hall Effect Based on m-Decomposed Density of State"

10:40- 11:20 Naoya Yamaguchi, "Implementation of Effective Potential for a Finite Electric Field Applicable to Bulk into OpenMX"

11:20-12:00 Monika Nur, "Surface Alloys on Noble Metal (111) Surfaces"

12:00-13:30 Lunch & Coffee break

13:30-14:10 Rifky Syariati, "Anomalous Nernst Effect in 2D Magnetic Materials"

14:10-15:00 Invited speaker: Dr. Hiroki Kotaka, "First-Principles Study of Battery Performance and Reaction Mechanism of Tin Sulfide as Negative Electrode"

15:00-15:30 Coffee break

15:30-16:10 Hikaru Sawahata, "Topological Insulators: Z₂ Topological Insulator and Chern Insulator"

16:10-16:50 Megumi Sugita, "The Rashba Effect in PbTiO₃/Ag"

16:50-17:30 Akihiro Hori, "Lattice Thermal Conductivity in Half-Heusler Alloys"

17:30 Closing Fumiyuki Ishii