

IBSPCS-APCTP International Workshop

Computational Approaches to Magnetic Systems

August 17 – 19, 2022

All times in the workshop program refer to Korean Standard Time (KST)

Program

Wednesday, August 17

09:30 – 10:30 Workshop Registration

10:30 – 10:45 Sergej Flach, PCS IBS
Opening address

10:45 – 11:30 Sonny Rhim, University of Ulsan, Korea
Nonvanishing anomalous Hall effect in Mn_3Al - compensated ferrimagnetic Heusler compound

11:30 – 12:15* Fumiyuki Ishii, Kanazawa University, Japan
First-principles Berry phase approach to magnetic systems (Online)

12:15 – 13:00 Workshop picture & Lunch

13:00 – 14:00 Discussions

14:00 – 14:45 Chang Jong Kang, Chungnam National University, Korea
Hidden Hund's Physics in the Infinite-Layer Nickelate Superconductors and Their Optical Properties

14:45 – 15:30* Tanusri Saha Dasgupta, S.N. Bose National Centre, India
A Tale of two Nickelates (Online)

15:30 – 16:00 Coffee Break

16:00 – 16:45 Atsushi Hariki, Osaka Metropolitan University, Japan
 $CaCu_3Ru_4O_{12}$: A High Kondo-Temperature Transition Metal Oxide

16:45 – 17:30* Gheorghe Lucian Pascut, Stefan Cel Mare Univ., Romania
Realistic Materials through the lens of embedded dynamical mean field theory (eDMFT) (Online)

17:30 – 18:15 Minjae Kim, KIAS, Korea
Emergent phase diagram of ruthenates: $SrRuO_3$ - $SrTiO_3$ heterostructure upon epitaxial strain

18:15 – 20:00 Welcome reception

Thursday, August 18

- 09:30 – 10:15 Aaram Kim, University of Fribourg, Switzerland
Pseudo-particle vertex impurity solver
- 10:15 – 10:45 **Coffee Break**
- 10:45 – 11:30 Kihoon Lee, Incheon National University, Korea
Exact diagonalization study of the Kitaev model under magnetic field
- 11:30 – 12:15 Heung-Sik Kim, Kangwon National University, Korea
Active orbital degree of freedom and potential spin-orbit-entangled moments in Kitaev magnet candidate $\text{BaCo}_2(\text{AsO}_4)_2$
- 12:15 – 13:00 **Lunch**
- 13:00 – 14:00 **Discussions**
- 14:00 – 14:45 Duck Young Kim, HPSTAR, China
High throughput computational study on Iron in the deep Earth
- 14:45 – 15:30* Peitao Liu, IMR CAS, China
On-the-fly machine-learned force fields generation and application: Density functional theory and beyond (Online)
- 15:30 – 16:00 **Coffee Break**
- 16:00 – 16:45 Turan Birol, University of Minnesota, USA
Real and Imaginary Charge Density Wave Phases in CsV_3Sb_5
- 16:45 – 17:30 Kyung Hwan Jin, IBS-CALDES, Korea
Tunable Mott Dirac and kagome bands engineered on 1T-TaS_2
- 17:30 – 18:15 Hong Chul Choi, IBS-CCES, Korea
Correlated normal state fermiology and topological superconductivity in UTe_2
- 18:15 – 20:00 **Workshop banquet**

Friday, August 19

- 09:30 – 10:15 Igor Di Marco, APCTP, Korea
Persistent half-metallic ferromagnetism in a (111)-oriented manganite superlattice
- 10:15 – 10:45 Coffee Break
- 10:45 – 11:30 Minsung Kim, UNIST, Korea
Correlation effects in layered systems FePS₃ and CrGeTe₃
- 11:30 – 12:15 Tae Yun Kim, IBS-CCES & Seoul National University, Korea
Magnetic anisotropy in transition-metal phosphorus trisulfides
- 12:15 – 13:00 Lunch
- 13:00 – 14:00 Discussions
- 14:00 – 14:45 Marco Battiato, Nanyang Technological Univ., Singapore
Emergence in out of equilibrium systems: from super diffusive spin transport to giant spin injection in semiconductors
- 14:45 – 15:30 Jae-Ho Han, PCS IBS
Magnetic interactions in Sr₂RuO₄ and superconducting gap symmetry
- 15:30 – 15:45 Scientific Coordinators
Closing remark