

理論セミナー / Theory Seminar

Date: July 9 (Fri.), 2021 16:00-
Place: On Zoom (Please make a registration through the link below)
Speaker: **Prof. Michi-To SUZUKI**
Affiliation: Institute for Materials Research, Tohoku University
Title: **Magnetic materials design by representation theory & first-principles calculation**

Abstract :

Diversity of physical properties of magnets provides a fascinating playground in condensed matter physics. What is interesting to note is that there are many restrictions for physical properties in magnets imposed by magnetic structure. It is often useful to represent some aspect of magnetic structure by using symmetry, order parameter, and topology. For example, it has been known that the finite elements of a linear response tensor are identified by the magnetic point group, which characterizes macroscopic symmetry of the magnetic structure.

Cluster multipole method is first suggested to identify the multipole order parameters related to anomalous Hall effect in antiferromagnets [1, 2] and is further developed to generate the orthonormal symmetrized magnetic structure bases providing multipole expansion for a given crystal structure [3]. The symmetrized magnetic bases are useful to produce high symmetric magnetic alignments which can be good candidates of stable magnetic structures for a magnetic compound. We recently applied the cluster multipole method combined with first-principles theory to investigate the transport phenomena of magnetic systems with predicting stable magnetic structures [4, 5] and established a framework to systematically evaluate the stable magnetic structures for given crystal systems [6]. In this talk, I introduce an overview of cluster multipole method and application to the study of magnetic compounds.

[1] Michi-To Suzuki, Hiroaki Ikeda, Peter M. Oppeneer, J. Phys. Soc. Jpn. **87**, 041008 (2018)

[2] M.-T. Suzuki, T. Koretsune, M. Ochi, R. Arita, Phys. Rev. B **95**, 094406 (2017)

[3] M.-T. Suzuki, T. Nomoto, R. Arita, Y. Yanagi, S. Hayami, H. Kusunose, Phys. Rev. B **99**, 174407/1-10 (2019)

[4] Vu Thi Ngoc Huyen, Michi-To Suzuki, Kunihiro Yamauchi, Tamio Oguchi, Phys. Rev. B **100**, 094426/1-9 (2019)

[5] Vu Thi Ngoc Huyen, Yuki Yanagi, Michi-To Suzuki, arXiv:2104.13704 (2021)

[6] M.-T. Huebsch, T. Nomoto, M.-T. Suzuki, and R. Arita, Phys. Rev. X **11**, 011031 (2021)



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