The Condensed Matter Theory / Computational Materials Science Seminar

CMT/CMS seminar

Date & Time: Oct 3rd (Thu.) 3:30pm -

Place: 6F small seminar rm, Sengen main bldg

Speaker: Dr. Hiroshi Shinaoka （品岡寛氏）

Institute for Theoretical Physics, ETH Zürich

Title: Spin-orbital frustration in pyrochlores $A_2Mo_2O_7$

Abstract:

Molybdenum pyrochlores $A_2Mo_2O_7$ have been investigated extensively because of their fascinating electronic and magnetic properties [1]. In particular, insulating compounds (A=Y, Tb, *etc.*) exhibit spin-glass behavior instead of conventional long-range ordering. However, the origin of the peculiar magnetic properties still remains to be clarified.

We study a typical insulating compound $Y_2Mo_2O_7$ by the fully relativistic density-functional theory plus on-site repulsion (U) method [2]. We determine the ground-state phase diagram with respect to U. We find peculiar competition in energy between different magnetic states in the large-U insulating region, which cannot be explained by simple Heisenberg antiferromagnetic spin models adopted in previous studies. We reveal that the system is in the competing region where anisotropic antiferromagnetic and ferromagnetic exchange interactions are competing with each other.

Analyzing a three-orbital Hubbard model, we clarify that the magnetic competition is tightly connected with orbital frustration in the $4d^2$ electronic configuration through the spin-orbital interplay. The results challenge the conventional picture of the spin-glass behavior that attributes the origin to the geometrical frustration of purely antiferromagnetic exchange interactions.

[1] J. S. Gardner, M. J. P. Gingras, and J. E. Greedan, Rev. Mod. Phys. **82**, 53 (2010).
[2] H. Shinaoka, Y. Motome, T. Miyake, and S. Ishibashi, arXiv:1305.0660.

Contact: MIYAZAKI.Tsuyoshi@nims.go.jp – Computational Materials Science Unit