

凝縮系物理学ゼミナール

Condensed Matter Seminar

Location: Room 413, School of Science Bldg. 5 (理学 5 号館 413 号室)

Time and date: 15:30 – 17:00, Monday, 30 September 2013

Spin-orbital frustration in pyrochlores $A_2Mo_2O_7$

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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 find peculiar competition in energy between different magnetic states in the large- U insulating region, which cannot be explained by simple Heisenberg antiferromagnetic 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.

References:

- [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.