First principles study on strong correlations in pyrochlore systems

Hiroshi SHINAOKA
Department of Physics, Saitama University, Saitama 338-8570, Japan

Pyrochlore systems exhibit fascinating phenomena emergent from electron correlations such as geometrically frustrated magnetism and spin-orbit physics. In this talk, we present our recent theoretical studies of $5d^5$ pyrochlore iridates [1] and the $3d$ spinel LiV_2O_4 [2].

In 2011, a Weyl semimetal was proposed as the ground state of some compounds in the series of $A_2Ir_2O_7$ (A=Pr, Nd, Y, *etc.*) [3], which stimulated further theoretical and experimental studies. However, due to experimental difficulties, the ground-state prosperities of the compounds remain to be clarified. We map out the low-temperature phase diagram by relativistic LDA+DMFT (local density approximation+dynamical mean-field theory) calculations. We show that the Weyl semimetal is unstable against strong electron correlations. We predict non-Fermi liquid behavior in hole-doped compounds. We discuss recent experimental results on hole-doped compounds.

The second half of the talk is devoted to the discussion of the origin of the heavy fermion behavior in the $3d$ spinel LiV_2O_4 [4]. This compound is the first example of $3d$ heavy fermion systems. There have been many theoretical proposals on its origin. Some of them focus on the role of geometrical frustration, inter-orbital hybridization, orbital-selective Mott physics. To achieve a consensus, we perform first-principles calculations of the compound at low T by means of LDA+DMFT method. We find the critical role of multi-orbital aspects. The t2g manifolds splits into an a_{1g} orbital with a smaller band width and doubly degenerate e'_g orbitals. The a_{1g} orbital stays slightly hole-doped ($0.8 < n_{a_{1g}} < 1$) in a wide parameter region near the realistic parameters estimated by the constrained RPA method. The heavy fermion state is stabilized in this wide region because of the emergence of the longer spin moments due to the Hunds coupling. We show that the heavy fermion state is robust against hole doping.

References

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