Project Title:

Electronic structure calculations for pyrochlore Ir/Rh oxides

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1. Possible topological phases due to the interplay between the electron correlation and the relativistic spin-orbit interaction in pyrochlore iridates have attracted great interest. Previous first-principles LDA+U calculations on $Y_2Ir_2O_7$ based on the LMTO method have revealed a possibility of realizing a cubic Weyl semi-metal phase with the broken time-reversal symmetry due to a so-called "all-in/all-out" non-collinear order of Ir magnetic moments. However, the non-collinear magnetism is quite often difficult to handle in a reliable manner, using currently available first-principle codes. Therefore, the magnetic ordering pattern and the associated possible topology have to be carefully examined by varying crystal parameters and Coulomb interaction strength and even substituting Ir with Rh. This is the main aim of the current work.
2. Electronic structures of pyrochlore iridates and rhodates have been investigated by performing fully relativistic first-principles calculations based on the OPENMX method for hypothetical $La_2M_2O_7$ (M = Ir, Rh) with RICC supercomputers. In particular, we mainly focused on the Ir case.
3. With varying lattice parameters as to mimic a lanthanide contraction in $R_2M_2O_7$ (R = Pr, Nd, Sm, and Eu) as well as an application of a hydrostatic pressure, we have obtained rough phase diagrams. A narrow-gap Z_2 topological band insulator has been obtained in the case with nearly regular MO_6 octahedra. We have also just started to include the on-site Coulomb repulsion for d electrons within the LSDA+U method. Our preliminary results show that it turns into a [100] ferromagnetic Mott insulator. With a moderately large trigonal distortion of MO_6 octahedra, we have obtained a band inversion and then a quadratic band touching at the Fermi level with a vanishing Fermi surface. Further increasing the trigonal distortion, We have also confirmed that the "all-in/all-out" magnetic order is stabilized by the on-site Coulomb repulsion, and then found an antiferromagnetic metal and antiferromagnetic insulator of this type.
4. The emergence of a ferromagnetic insulator in $R_2Ir_2O_7$ is our remarkably new finding, which might be accessible under strong hydrostatic pressure. We also observed a band-inversion transition from Z2 topological insulator to a quadratic band touching semimetal and then to a metal, with increasing a trigonal distortion of IrO_6 octahedra.
5. It remains open to establish the whole phase diagram in the space of the lattice parameters and the on-site Coulomb interaction. Also, it will be intriguing to identify the nontrivial topology in the ferromagnetic insulator phase. These will be issues left for the next fiscal year project.

Fiscal Year 2013 List of Publications Resulting from the Use of RICC

[Oral presentation at an international symposium]

"First-Principles study on pyrochlore iridates and rhodates: metal-insulator transition, magnetism, and topology"

(Invited talk at Workshop on Frustration and Topology in Condensed Matter Physics, Tainan, Feb. 14-16, 2014)

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