

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Electron interactions, spin-orbit coupling, intersite correlations in pyrochlore iridates: a comparison of single-site and cluster calculations¹

RUNZHI WANG, Columbia University, ARA GO, Institute for Basic Science, ANDREW MILLIS, Columbia University — Pyrochlore iridates ($R_2Ir_2O_7$) are studied using density functional theory plus single-site and cluster dynamical mean-field theory (DFT+DMFT). The calculations include spin-orbit coupling. Significant differences between the single-site and cluster calculations are found. The single-site approximation fails to account for the properties of the paramagnetic insulator phase, in particular predicting a larger gap than found in experiments, while cluster calculations yield gaps consistent with transport data. A ground-state phase diagram is computed. Paramagnetic metal, metallic all-in/all-out (AIAO) and insulating AIAO phases are found. Tilted Weyl cones are observed in the AIAO metallic phase for a relatively wide range of interaction strength. Our paramagnetic calculations predict almost identical behaviors for the Y and Eu compound, conflicting with the strong material dependence reported in experiments. Inclusion of magnetic order restores the material difference. The physical origin of the difference is discussed. The results indicate that intersite effects, most likely of antiferromagnetic origin, play an important role in studying the physics of pyrochlore iridates.

¹This work is supported by DOE-ER046169.

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Date submitted: 10 Nov 2016

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