

Abstract Submitted
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Interplay of many-body and single-particle interactions in iridates and rhodates¹ YURIY SIZYUK, NATALIA PERKINS, Univ of Minn - Minneapolis, PETER WOLFLE, Institute for Condensed Matter Theory and Institute for Nanotechnology, Karlsruhe Institute of Technology — Motivated by recent experiments exploring the spin-orbit-coupled magnetism in $4d$ - and $5d$ -band transition metal oxides, we study magnetic interactions in Ir- and Rh-based compounds. In these systems, the comparable strength of spin-orbit coupling (SOC), crystal field splitting (CF) and Coulomb and Hund's coupling leads to a rich variety of magnetic exchange interactions, leading to new types of ground states. Using a strong coupling approach, we derive effective low-energy super-exchange Hamiltonians from the multi-orbital Hubbard model by taking full account of the Coulomb and Hund's interactions in the intermediate states. We find that in the presence of strong SOC and lattice distortions the super-exchange Hamiltonian contains various kinds of magnetic anisotropies. Here we are primarily interested in the magnetic properties of Sr_2IrO_4 and $\text{Sr}_2\text{Ir}_{1-x}\text{Rh}_x\text{O}_4$ compounds. We perform a systematic study of how magnetic interactions in these systems depend on the microscopic parameters and provide a thorough analysis of the resulting magnetic phase diagram. Comparison of our results with experimental data shows good agreement.

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