Theoretical study of electronic structure and magnetic property of $URhIn_5$

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Over the last twenty years, heavy fermion compounds from the '115' family have attracted growing experimental attention. These materials follow a XYZ_5 composition, with a lattice structure that can be considered as a particular intermediate between the ``infinite layer'' $XZ_3$ geometry of their parent compound, and the ``double layer'' case with composition: X_2YZ_8. Initial interest in studying material properties upon adding the Y transition metal was prompted by the evolution of superconducting temperature with applied pressure, or with the change from a cubic unit cell into a tetragonal arrangement; and spin/charge correlation analogies with examples from the cuprate family [1].

Experimentally, one notes the appearance of superconductivity when X=Ce or Pu, and its absence when X=U or Np. This difference has been related to the localized vs. itinerant nature of the f electrons, and prompted a variety of experimental investigations [2].

Our work focuses on the $URhIn_5$ example, characterized by an electronic specific heat coefficient of 50 (mJ/K^2mole), and a Néel temperature of 98 (K) [3] with a $\mathbf{Q}$=(1/2,1/2,1/2) AF ground state determined by nuclear quadrupole resonance and neutron scattering experiments [4].

In order to support experimental interpretation, electronic structure calculations have been performed at different levels: from qualitative reconstructions [5] model Hamiltonian studies [6] to fully first-principles investigations based on density functional theory (DFT) and its possible extensions to better account for correlation effects. In general, a reliable description of 115 materials needs to address various aspects: strong spin-orbit due to the heavy lanthanides/actinides atom X, satisfactory treatment of f electrons, and accurate description of magnetism.

In general, the most comprehensive scheme to handle these aspects works at the level of an all-electron, Dirac equation -based framework, and we present here preliminary results obtained via the Munich Spin Polarized Relativistic Korringa, Kohn, Rostoker (SPRKKR) multiple scattering package [7], to compare predicted electronic structure and magnetic properties with available experiments.

Reference

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