Understanding strong-correlation effects in spin-orbit t_{2g} materials

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Strong-correlation effects in systems with low symmetry, non-spherical Coulomb vertex and spin-orbit interaction are particularly difficult to describe. Recent advances make it possible to investigate these phenomena via QMC-based LDA+DMFT calculations [1]. In this talk, I will use this technique to explain the electronic properties of representative t_{2g} materials [1-5]. For the unconventional superconductor Sr_2RuO_4 i will clarify the key role played by spin-orbit coupling and tetragonal Coulomb terms in determining the topology of the Fermi surface. For the Mott insulator Ca_2RuO_4, I will show that the spin-orbit interaction plays a little role in the metal-insulator transition. For the magnetic phase, two different scenario have been proposed, the local spin-moment ($S = 1$) scenario and the zero total-angular-momentum (or van-Vleck) picture. I will show that magnetic order and spin-wave spectra are well described in the perturbative spin-orbit limit, thus excluding the van-Vleck scenario.

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