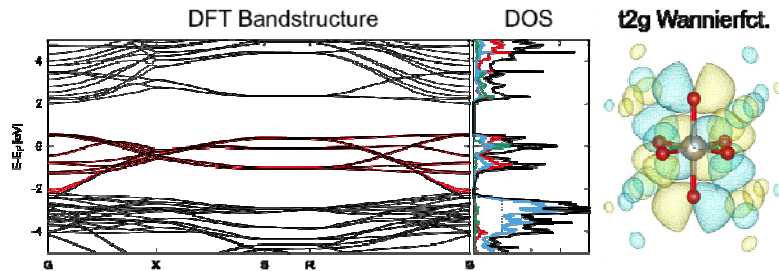


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| Quantum Magnetism in Materials with Strong Correlations and Spin-Orbit coupling 14GS | | Start Date: January 1 st 2017 |
| PhD: Michael Schmid (Stuttgart) | PIs: M. Daghofer (Stuttgart) P. Hansmann (MPI) | |
| <p>Abstract: We plan to investigate material properties driven by quantum effects in systems with strong spin-orbit coupling and substantial correlations, in particular compounds with 4 electrons in the most relevant t_{2g} orbitals (iridates or ruthenates) [1].</p> <p>Current interest in iridates is mainly due to the interplay of spin-orbit coupling, correlations and potential topologically nontrivial states. Most of the focus has so far been on materials with 5 t_{2g} electrons, with the hole in a state with total angular momentum $j=1/2$. Mainly two issues are of interest: (i) Magnetic interactions in honeycomb-lattice iridates are very direction dependent and have been proposed as a realization of Kitaev's spin liquid with anyonic excitations [2]. (ii) Square-lattice iridates can be modelled with a one-band Hubbard model similar to high-T_C cuprate superconductors [1,3,MD2,MD4]. In both cases, the motivation comes from the strong quantum effects expected for small angular momentum together with the specific manifestations of orbital-driven anisotropies. Especially the physics of honeycomb compounds, but also that of square lattices [MD4,MD5], has moreover been shown to be rather sensitive to material-specific aspects like additional (longer-range) couplings and crystal distortions.</p> <p>The project aims to combine numerical methods available to various groups at the MPI and university to arrive at a unified realistic picture. Additionally, methods will be extended.</p> | | |
| <p>Recent results:</p> <ul style="list-style-type: none"> <i>Ab initio bandstructure calculations and Wannier projections for spin orbit coupled systems: Ruthenates (Ca₂RuO₄, Sr₂RuO₄)</i>  <p>Ca₂RuO₄: Bandstructure, single particle DOS, and one of the Ru t_{2g} Wannier functions</p> | <p>Publications:</p> <ul style="list-style-type: none"> DMFT study of Ca₂RuO₄ (planned) Novel FCIQMC impurity solver for DMFT (planned) DMFT study for Ce based Heavy Fermion systems (planned) | |
| <p>Further Collaborators:</p> <p>A. Alavi (MPI-FKF: FCIQMC project) K. Guther (MPI-FKF: FCIQMC project) D. Mantadakis (MPI-FKF: Heavy Fermion DMFT project) M. Kim (College de France: Ruthenate project)</p> | | |