IQ ST Integrated Quantum Science and Technology

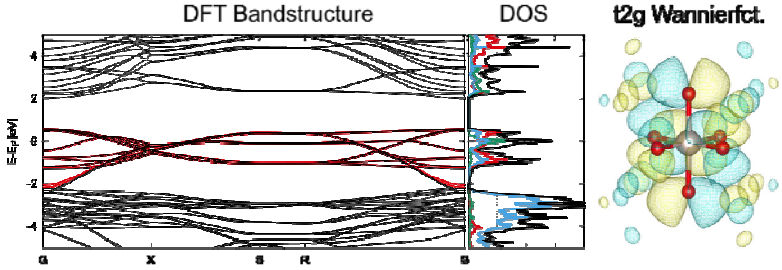
University of Stuttgart Germany | ulm university universität ulm | Max Planck Institute for Solid State Research

Quantum Magnetism in Materials with Strong Correlations and Spin-Orbit coupling | 14GS	**Start Date:** January 1st 2017
PhD: Michael Schmid (Stuttgart)	**PIs:** M. Daghofer (Stuttgart) P. Hansmann (MPI)

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].
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.
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.

Recent results:

- *Ab initio bandstructure calculations and Wannier projections for spin orbit coupled systems: Ruthenates (Ca2RuO4, Sr2RuO4)*



Ca2RuO4: Bandstructure, single particle DOS, and one of the Ru t2g Wannier functions

- *Implementation of state-of-the-art quantum chemical methods (FCIQMC) as impurity solver for dynamical mean-field theory (collaboration with AG Alavi)*
- *Supporting calculations for Ce based Heavy Fermion compounds (CeX2Si2)*

Publications:

- DMFT study of Ca2RuO4 (planned)
- Novel FCIQMC impurity solver for DMFT (planned)
- DMFT study for Ce based Heavy Fermion systems (planned)

Further Collaborators:
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)