CORRELATION-DRIVEN WEYL PHYSICS FROM AB INITIO DFT+DMFT THEORY

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Strongly correlated materials provide a platform for emergent quantum phases [1], including heavy-fermion metals, Kondo insulators, and unconventional superconductors. These phases arise from the interplay between crystal symmetries and complex many-body effects. Describing them from first principles is particularly challenging, as conventional density functional theory (DFT) fails to capture the low-energy quasiparticle physics. Here, using **state of the art** DFT combined with dynamical mean-field theory (DFT+DMFT) [2], we investigate the f-electron heavy-fermion compound $CeRu_4Sn_6$ to resolve its electronic structure and topology.

Our calculations show that Kondo hybridization opens a direct gap in the electronic structure, which is bridged by topological band crossings (Weyl nodes) along low-symmetry directions. We identify five inequivalent Weyl nodes of both type-I and type-II, generating a total of 64 symmetry-related Weyl points. A comprehensive analysis of these correlation-driven Weyl features is presented in our recent work [3]. The Weyl nodes emerge within correlated quasiparticle bands mainly composed of Ce-$4f$ orbitals and exhibit small electron velocities close to the Weyl nodes (below 10 km/s). The nodes closest to the Fermi energy lie approximately 0.5 meV below E_{F}, placing the Weyl physics at experimentally accessible energy scales.

These *ab initio* results establish $CeRu_4Sn_6$ as a model system for correlation-driven Weyl physics in f-electron materials, highlighting the importance of many-body correlations in $CeRu_4Sn_6$ and heavy-fermion systems in general. More broadly, this work provides a foundation for understanding interaction-driven topological phases and quantum transport phenomena in correlated quantum materials.

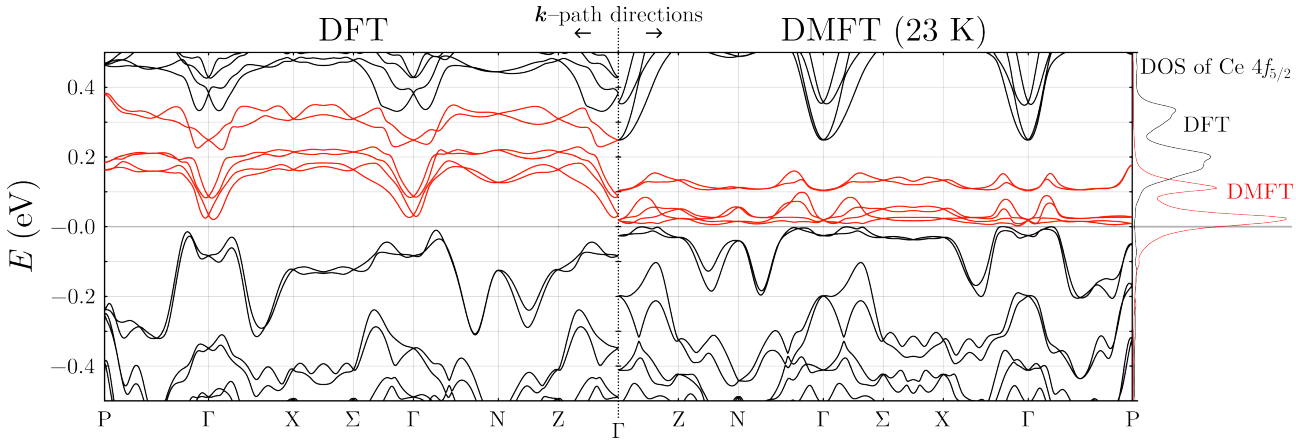

Fig. 1. Mirrored band structures of $CeRu_4Sn_6$ from DFT (left) and DFT+DMFT at 23 K (right) along identical high-symmetry paths centered at Γ. The Ce $f_{5/2}$ manifold is highlighted with red color to emphasize how Kondo hybridization reshapes the electronic structure. Correlation effects, included in DMFT solution, generate additional avoided band crossings and node-like features in the lower bands that are absent in DFT, revealing traces of Weyl physics. The side panel shows the corresponding Ce $4f_{5/2}$ density of states, confirming the emergence of Kondo effect at the Fermi level.

Keywords: Topology, Weyl Physics, DFT+DMFT

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