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Calculated electronic structure properties of URu_2Si_2 and Ce-115 materials

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The Ce-115 materials are archetypal heavy-fermion superconductors that display a fascinatingly rich interplay of magnetism and superconductivity. We employ density-functional theory (DFT) based calculations to approach the correlated f-electronic structure of these materials. In particular, we compute the nuclear quadrupole resonance (NQR) frequencies at the In-sites in pure and Cd-, Sn- doped Ce-115's and compare with recent experiments. The degree of Ce $4f$-localization is treated through the application of various models (local density approximation, generalized gradient approximation, GGA+U, and f-core approach). We find that there is a correlation between the NQR and Ce $4f$-behavior. In another collaboration we use ARPES to study the Fermi surface of the Kondo lattice material $CeCoIn_5$ halfway the lattice coherence temperature (T*$\sim$45 K) and compare with DFT calculations. We find that at T=26 K the Fermi surface of $CeCoIn_5$ is not enlarged, implying that signatures of coherence in the transport data can develop without a concomitant enlargement of the Fermi surface. We furthermore investigate URu_2Si_2 which hidden order (HO) phase has been a mystery for many years and provide a microscopic explanation for the HO. We identify the Fermi surface "hot spots" where degeneracy induces a Fermi surface instability and quantify how symmetry breaking lifts the degeneracy, causing a surprisingly large Fermi surface gapping. We show that our electronic structure model is fully consistent with all known experimental properties of URu_2Si_2.