DFT-L(S)DA simulations for URu_2Si_2 and UCu_2Si_2

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The two heavy fermion systems, superconducting URu_2Si_2 and ferromagnetic UCu_2Si_2, represent two intermetallic compounds of similar structure and astonishingly different electronic and magnetic properties. Recognition of the degree of localization of f-electrons and the extend to which the *f* electrons contribute to the Fermi surface topology are of crucial importance for their understanding. Over 20 years of intensive investigations and discussions on the mysterious ordered phase observed in URu_2Si_2 below 17.5 K gives an idea about the scale of difficulties [1]. Strong correlations of electrons on the threshold of becoming localized are essential in these materials. Their actual discussion requires detailed information about the ongoing one-electron structure. In the light of the known limitations of the developed methods of *ab initio* calculations based on density functional theory and the local density approximation, this is not a trivial task.

The presented here results of series of DFT-L(S)DA calculations for the compounds under consideration have been obtained using the FPAPW and FPLO procedures [2]. Both the relativistic and non-relativistic versions of the latter method have been taken into account. The spin polarization and other extensions have been probed together with a variation of some initial parameters in order to check the stability of the solutions and to imitate external pressure or magnetic field. The calculations correctly predict the main characteristics of the materials, verifiable within the DFT approach, in particular, the ferromagnetic ordering for UCu_2Si_2 and nonmagnetic ground state for the second example.

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