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Angle-resolved Photoemission of CeCoIn₅: Detailed Comparison to LDA and LDA+DMFT

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Highly-automated photon-dependent angle resolved photoemission spectroscopy (ARPES) in the energy range of 80-200 eV has been used to characterize the three dimensional (3D) Fermi surface (FS) topology and electronic band structure of cleaved single crystals of CeCoIn₅. The sample temperature of $\approx 26\text{K}$ is well below the lattice coherence onset temperature of $\approx 45\text{K}$ found in a recent “two fluid” analysis of transport data. Detailed comparison of ARPES FS contours to LDA calculations for the Ce 4f electrons treated as itinerant or confined to the core reveals remarkable agreement to fine topological details of the f-core calculations. Also in agreement to the f-core calculations is the experimental absence of extra electron-like contours predicted in the f-itinerant calculation, originating from α and β bands re-entrant below E_F along Z-A. Finally, the areas enclosed by FS contours for the α and β bands are significantly smaller than are found in very low temperature CeCoIn₅ de Haas van Alphen data that agrees generally with the f-itinerant calculation. It is concluded that clear signatures of coherence in the transport data can develop at temperatures for which the f-electrons are not yet included in the FS. In this connection, comparison will also be made to recent T-dependent LDA+DMFT calculations for CeIrIn₅. This work was done in collaboration with J. D. Denlinger, Feng Wang, R. S. Singh, K. Rossnagel, S. Elgazzar, P. M. Oppeneer, V. S. Zapf and M. B. Maple, and was supported by the U.S. DOE (DE-AC03-76SF00098 at the ALS, DE-FG02-07ER46379 at UM for current work, DE FG02-04ER-46105 at UCSD), by the U.S. NSF (DMR-03-02825 at UM for initial work, DMR-03-35173 at UCSD) and by the Swedish Research Council (VR) and the European Commission (JRC-ITU).