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Three-dimensional band structure of heavy fermion CeCoIn5 measured by photon-dependent angle resolved photoemission

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Photon-energy dependent angle-resolved photoemission spectroscopy (ARPES) is used to map the 3D band structure and Fermi Surface of the archetypal Kondo lattice material, CeCoIn5. ARPES measurements from two different <001> and <100> cleave surfaces give complementary orthogonal views of the electronic structure with photon-energy dependent kz-broadenings in different crystallographic momentum directions, thereby partially overcoming an inherent ARPES limitation for three-dimensional systems. Polarization dependence of 4d-4f resonantly-excited ARPES is then used to help identify the k-locations of high Ce 4f spectral weight. Detailed comparison is made to local density functional (LDA) calculations in which the Ce 4f-electrons are treated as part of the conduction electrons or as unhybridized localized core states. Clear overall agreement to the localized LDA calculation is observed for all binding energies up to the very low energy scale near EF where signatures of f-d hybridization are observed. However some high binding energy scale disagreement with LDA also exists for CeCoIn5, but not for CeRhIn5 and CeIrIn5, and indicates the need for improved theoretical treatment of Co 3d electron correlations relative to the 4d and 5d systems. The resulting detailed experimental knowledge of the full 3D band structure, k-locations of strong f-d hybridization, and differences between 3d, 4d and 5d Ce115 systems are key steps towards verifying the recent LDA+DMFT predictions of the temperature-dependent Fermi surface evolution in CeIrIn5 [1].

[1] H. C. Choi, B. I. Min, J. H. Shim, K. Haule and G. Kotliar, Phys. Rev. Lett. 108, 016402 (2012).

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