Title:

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from ARPES**

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The Electronic Structure of CeRhIn₅ and LaRhIn₅ from ARPES

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Abstract

In the heavy fermion CeRhIn₅ and the isostructural compound LaRhIn₅ the extra 4f electron in Ce dramatically alters the band structure near E_F, suggesting that the 4f's participate in band formation. ARPES data indicates that correlation effects are mostly evident along the Γ -Z direction in the Brillouin zone. Very good agreement to GGA band calculations is found.

Keywords

CeRhIn₅, photoemission, band structure

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The discovery [1,2] of a new class of heavy fermion superconductors (CeMIn_5 , $\text{M}=\text{Co,Rh,Ir}$) has generated much activity investigating their low temperature magnetic and electronic properties. An ordered magnetic or superconducting state is obtained at low hydrostatic or ambient pressure, while specific heat γ -values range from 250 to 750 mJ/mole- K^2 . They represent the heaviest Ce heavy electron systems to undergo a superconducting transition since the discovery of CeCu_2Si_2 . The electronic structure and effects of correlations are best studied by angle-resolved photoemission (ARPES).

Here we focus on the electronic structure of the heavy fermion CeRhIn_5 and isostructural LaRhIn_5 with ARPES. The crystal structure for both compounds is tetragonal [3] with lattice constants of $a_0=4.656\text{\AA}$, $c_0=7.542\text{\AA}$ for Ce and $a_0=4.672\text{\AA}$, $c_0=7.602\text{\AA}$ for La. They can be viewed as layered, with units of Ce(La)In_3 separated by units of RhIn_2 . It has been suggested [1] that it is the two-dimensional layers of CeIn_3 which govern the unusual properties in this heavy fermion compound.

ARPES measurements were performed at the Synchrotron Radiation Center using the Ames-Montana beam line and an HA50 analyzer with the pressure in the Ames spectrometer chamber maintained below 5×10^{-11} Torr. Single crystals were grown via the flux growth technique. Samples were epoxied to a cold finger of a cryostat, cleaved in vacuum, and measured at $T \sim 15$ K. Although substantial off-axis data exists, we focus on normal emission data (i.e., electrons emerging from the cleaved a-b plane along the c-axis) obtained by varying the photon energy from about 10 eV to about 100 eV.

The data are presented in Fig. 1 where panels A, B and D are the reduced ARPES data representing the experimentally determined band structure for CeRhIn₅ (A and B) and LaRhIn₅ (D). Panel C shows the calculated bands for CeRhIn₅ along Γ -Z using the generalized gradient approximation (GGA) within density functional theory. The left-most panel (A) shows off-axis CeRhIn₅ data (nominally along the Γ -M direction) obtained at varying emission angles of the outgoing electrons. We utilized free electron final states for normal emission analysis, and determined an inner potential of 8.7 eV.

Comparing panel B with panel C we notice that for energies lower than ~ -1.5 eV there exists a strong similarity between the calculated and experimental bands. Indeed, even the band structure of LaRhIn₅ appears to be very similar in this range. The minor discrepancies below -4 eV are not significant since the calculation was optimized near E_F . The most serious discrepancy occurs near the Z-point at ~ -2.5 eV where an apparent unpredicted band exists. We believe this to be the usual 4f satellite (commonly referred to as the bare f-peak) observed in most Ce materials. It is concluded that there is no renormalization of bands below -1.5 eV due to correlation effects and agreement with GGA is very good.

The effects of f-electron correlations are strongly evident in the bands near E_F , labeled *a*, *b*, *c*, and *d* in Fig.1. For these bands GGA predicts a strong f-admixture. They are substantially narrowed relative to GGA, with bands *a* and *b* (greatest f-admixture) becoming nearly flat along Γ -Z and pulled below E_F . They still retain some p- or d-character, however, particularly away from the Γ -Z direction, based on cross-section dependence. To within experimental resolution, band *a* is actually situated at the Fermi energy. The lack of

dispersion in band a is consistent with a heavy electron mass and is likely responsible for the heavy fermion behavior. Comparing panels B and D, the addition of one 4f-electron dramatically alters the electronic structure and Fermi surface (most obvious for band b). Thus the 4f-electrons hybridize, participate in the band structure, and have 4f-weight distributed throughout bands a and b , less in c and d .

Turning to panel A (Γ -M direction), we see that bands a and b disperse by as much as 1 eV. This is highly unusual [4] for 4f-bands in a material having a γ -value of 400 mJ/mole-K². Indeed, it represents the largest f-band dispersion ever observed in a heavy fermion. On the other hand, bands a , b , c , and d are in much better agreement with GGA along Γ -M than along Γ -Z. This suggests that most of the correlation effects occur along Γ -Z in the Brillouin zone. This flattening of the 4f-bands along Γ -Z has the effect of inducing a *de facto* two-dimensionality for the f-bands only, while the remaining bands retain a three-dimensional structure. This point is further emphasized by the observation that bands a through d in isostructural LaRhIn₅ (panel D) are highly dispersive, indicative of a normal three-dimensional crystal structure. The quasi-two-dimensional f-band structure in CeRhIn₅ is thus primarily a consequence of correlations. An additional interesting feature of the Ce 4f spectra is the surprisingly weak 4f intensity, both at resonance and at lower photon energies where the 4f intensity should dominate. The large dispersion may play a role.

Qualitative differences in band structures of LaRhIn₅ and CeRhIn₅ suggest that despite the heavy fermion nature of CeRhIn₅ the 4f electrons participate in bonding. The correlation effects are most evident along Γ -Z where the hybridized 4f-bands are nearly flat, but highly

dispersive elsewhere, thus yielding a *de facto* two-dimensional 4f band structure. Other band symmetries remain three-dimensional. In general, there is excellent agreement with GGA band calculations.

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References

1. H. Hegger, et al., Phys. Rev. Lett. 84 (2000) 4986.
2. C. Petrovic, et al., Europhys. Lett. 53 (2001) 354.
3. E.G. Moshopoulou, et al., J. Solid State Chem. 158 (2001) 25.
4. A.J. Arko, et al., Handbook on the Physics and Chemistry of the Rare Earths, ed. K.A. Gschneider and L. Eyring (Elsevier, New York, 1999) Vol.26, pp 265-38.

Figure Caption

Fig.1. Reduced ARPES data (points) for CeRhIn₅ (panels A and B) and LaRhIn₅ (panel D) with lines as guides to the eye. GGA results are in panel C.