

TIGHT-BINDING MODEL FOR HEAVY FERMION COMPOUNDS: CONSTRUCTION OF f - p MODEL*

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We discuss electronic properties of CeIrIn_5 based on the relativistic band-structure calculation. The obtained energy band-structure is reanalyzed by using a tight-binding f - p model, which is found to be a realistic and practical Hamiltonian for CeTIn_5 ($T = \text{Ir, Rh, and Co}$).

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Recently Ce-based heavy fermion superconductors CeTIn_5 ($T = \text{Ir, Rh, and Co}$) have attracted much attentions in the research field of strongly correlated electron systems [1]. The so-called Ce-115 compound has the HoCoGa_5 -type tetragonal crystal structure with alternating layers of CeIn_3 and TIn_2 stacked along the $[001]$ direction, as shown in Fig. 1(a), indicating that two-dimensionality is strong in this material. In fact, the angular dependence of major experimental de Haas-van Alphen frequency branches is well explained by quasi two-dimensional Fermi surfaces [2].

Due to the simple two-dimensionality of the Fermi surfaces and magnetic property, CeIrIn_5 is an ideal example for fundamental study of superconductivity and magnetism in rare earth compounds. However, when we attempt to promote such an investigation for CeTIn_5 from a microscopic viewpoint, we encounter a problem of absence of an appropriate Hamiltonian for the f electron systems. Thus, we will try to construct a microscopic model by combining the band calculation and the tight-binding method.

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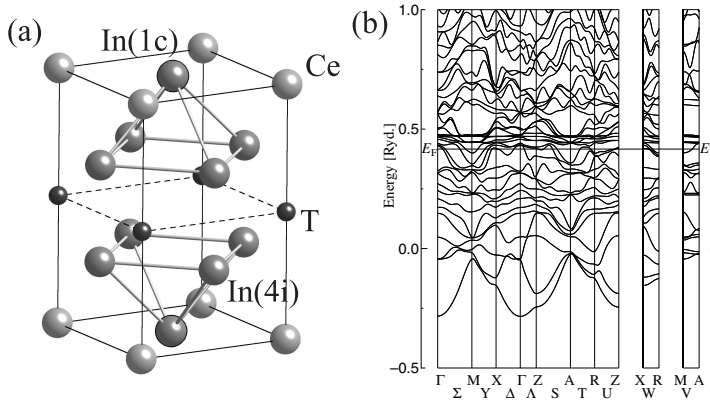


Fig. 1. (a) Crystal structure of CeTiIn₅. (b) Energy band structure calculated for CeIrIn₅ with the RLAPW method.

In this paper we first discuss electronic properties of CeIrIn₅ from the band calculation within the local density approximation (LDA). Second we reanalyze the energy band structure in comparison with a tight-binding model including Ce 4*f* and In 5*p* states. The overall framework of the band structure around the Fermi energy E_F is determined by the broad *p* band and *f*-*p* hybridization, while the fine structure in the vicinity of E_F is sensitive to the narrow *f* bands and crystalline electric field (CEF) effects.

Let us briefly discuss the energy band structure calculated by using the relativistic linear augmented plane wave (RLAPW) method with the exchange and correlation potential in the LDA. The muffin-tin approximation is adopted for the spatial shape of one-electron potential and self-consistent calculations are carried out for experimental lattice constants. In the calculated energy band structure for CeIrIn₅, as shown in Fig. 1(b), four characteristic features are observed: (i) $E_F = 0.416$ Ryd. in the present unit and 13th–16th bands construct the Fermi surfaces. (ii) Around E_F , hybridization between Ce 4*f* and In 5*p* states occurs. (iii) Above E_F near the *M* point, flat 4*f* bands split into two groups, specified by $j = 5/2$ for lower and $7/2$ for upper bands, respectively (j is the total angular momentum). (iv) The magnitude of the splitting in 4*f* states corresponds to the spin-orbit coupling, estimated as 0.4 eV.

As suggested in the point (iii) above, energy bands around E_F are composed of $j = 5/2$ states. Thus, we take into account only the $j = 5/2$ sextet to construct an effective model for low-energy excitations. Moreover, since the Fermi surfaces exhibit two-dimensionality both in experiments and in the band calculation, we consider the tight-binding model within the $j = 5/2$ sextet on the two-dimensional lattice shown in Fig. 2(a).

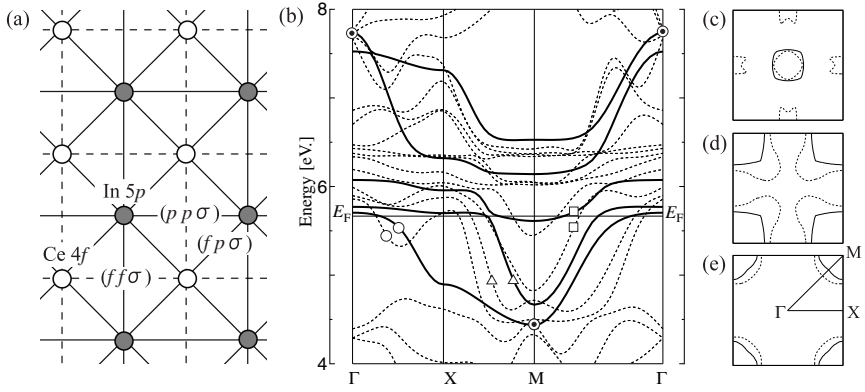


Fig. 2. (a) Two-dimensional lattice composed of Ce (open circles) and In (gray circles) ions. (b) Energy band structures around E_F for CeIrIn₅. Solid and dashed curves indicate the results for f - p model and the RLAPW calculation, respectively. Circled dots denote top and bottom of tight-binding bands. Pairs of circles, triangles, and squares indicate correspondence between the RLAPW and tight-binding bands. Fermi-surface lines discussed here are (c) 13th band hole sheets, (d) 14th band hole sheets, and (e) 15th band electron sheets.

Due to the lack of space, we skip detailed explanations for the tight-binding procedure, but here only the result is shown:

$$H = \sum_{\mathbf{k}\mu\nu\sigma} [(\varepsilon_{\mathbf{k}\mu\nu}^f + \Delta_{\mu\nu}^f) f_{\mathbf{k}\sigma\mu}^\dagger f_{\mathbf{k}\sigma\nu} + (\varepsilon_{\mathbf{k}\mu\nu}^p + \Delta_{\mu\nu}^p) p_{\mathbf{k}\sigma\mu}^\dagger p_{\mathbf{k}\sigma\nu} + V_{\mathbf{k}\mu\nu} (f_{\mathbf{k}\sigma\mu}^\dagger p_{\mathbf{k}\sigma\nu} + \text{h.c.})],$$

where $f_{\mathbf{k}\sigma\mu}$ ($p_{\mathbf{k}\sigma\mu}$) is an annihilation operator for f (p) electron with momentum $\mathbf{k}$ and pseudo-spin σ in the μ orbital. Note here that $f_{\mathbf{k}\sigma\mu}$ is given by the linear combination of the states in the $j = 5/2$ sextet, while $p_{\mathbf{k}\sigma\mu}$ is composed of the states in the $j = 1/2$ doublet and $j = 3/2$ quartet. The dispersion energies for f and p electrons are given by $\varepsilon_{\mathbf{k}\mu\nu}^f$ and $\varepsilon_{\mathbf{k}\mu\nu}^p$, respectively, while $V_{\mathbf{k}\mu\nu}$ indicates f - p hybridization. Effects of tetragonal CEF are included in $\Delta_{\mu\nu}^f$ and $\Delta_{\mu\nu}^p$ for f and p electrons, respectively. Parameters in H are three Slater integrals $[(f p \sigma), (p p \sigma), (f p \sigma)]$ and several CEF parameters, which are determined so as to be consistent with the band calculation results.

In Fig. 2(b) we show a typical result for comparison between the RLAPW and the tight-binding energy bands. For a given value of $(f f \sigma)$, we determine $(p p \sigma)$ and $(f p \sigma)$ in a manner that energies at the top and bottom of tight-binding bands are just equal to those at the Γ point of the 25th band and at the M point of the 12th in the RLAPW result, respectively, since those bands

originate from In $5p$ states. Then, we obtain $(pp\sigma) = 7010\text{ K}$ and $(fp\sigma) = 11280\text{ K}$ for $(ff\sigma) = 2000\text{ K}$ [3]. CEF parameters have been determined in the f - f model without p electrons [4]. Details of parameter fitting as well as the derivation of H will be discussed elsewhere [5].

Here we focus on the three Fermi surfaces constructed from 13th, 14th, and 15th bands in the RLAPW result, since f and p components in the 16th-band Fermi surface are quite small. The tight-binding model has several bands crossing E_F along the Γ - M and X - M ions, reproducing two large cylindrical sheets corresponding to the 14th- and 15th-band Fermi surfaces in the RLAPW result, as shown in Fig. 2 (d) and (e). We can also reproduce a portion of the small 13th-band Fermi surfaces, as shown in Fig. 2(c), which could not be obtained in the f - f model [4]. Thus, it is suggested that the Fermi surfaces of the f - p model agree well with the RLAPW results.

In summary, the energy band and Fermi surface structures of CeIrIn_5 have been discussed by combining the band calculation and the tight-binding f - p model. The Fermi surface topology in the f - p model is consistent with the band calculation and experimental results. We believe that the f - p model may serve as a realistic Hamiltonian to discuss magnetism and superconductivity in CeTIn_5 by further adding Coulomb interaction terms.

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