(PS8)

Tight-binding Band with T_h Symmetry and the Electronic Structures of Ce- and Pr-Skutterudites

T. Saso and Y. Imai

Department of Physics, Saitama University, Saitama-City, 338-8570

It is important to construct a simple tight-binding band for the skutterudite compounds to consider the effect of strong correlations. We have previously found that the energy dispersions of some Ce-skutterudite compounds can be understood rather well as the basic p-electron valence band of the HOMO of pnictogen X_{12} clusters (similar to the s-band on the bcc lattice) plus the 4f bands above it.[1] There is a strong hybridization between the HOMO band and the 4f states. In the electronic structures of some insulating compounds (Kondo insulators) may be understood in terms of this model if we place the Fermi energy between the HOMO and the 4f bands.[1] In the case of La- and Pr-compounds, E_F lies in the middle of the HOMO band. In the latter case, almost localized f^2 ($J = 4$) electrons are sunk in a deep position.

In the present study, we have included the necessary crystal field potential $\mathcal{H}_{CEF}(T_h)$ of the local T_h symmetry, which was neglected and replaced by that of O_h in the previous study.[1]

$$\mathcal{H}_{CEF} = \mathcal{H}_{CEF}(O_h) + \mathcal{H}_{CEF}(T_h),$$

$$\mathcal{H}_{CEF}(O_h) = W\left[x\frac{O_4}{F(4)} + (1-|x|)\frac{O_6^c}{F(6)}\right], \quad \mathcal{H}_{CEF}(T_h) = Wy\frac{O_6^t}{F_t(6)} \tag{1}$$

$\mathcal{H}_{CEF}(T_h)$ operates only on the Γ_6 and Γ_7 states of J=7/2 under O_h symmetry, which lie at rather high energy. The tight-binding band is constructed by the linear combination of the CEF eigenstates $\phi_{i\alpha}$. In order to fit the LDA bands, the energy levels under $\mathcal{H}_{CEF}(O_h)$ are chosen as the free parameters instead of x and W. The increase of y results in the larger splitting of $\Gamma_5^{(1)}$ and $\Gamma_5^{(2)}$ states.

Many-body effects may be taken into account in the same manner for Ce and Pr compounds as in the previous study[1] at least if one uses the $j-j$ coupling scheme.

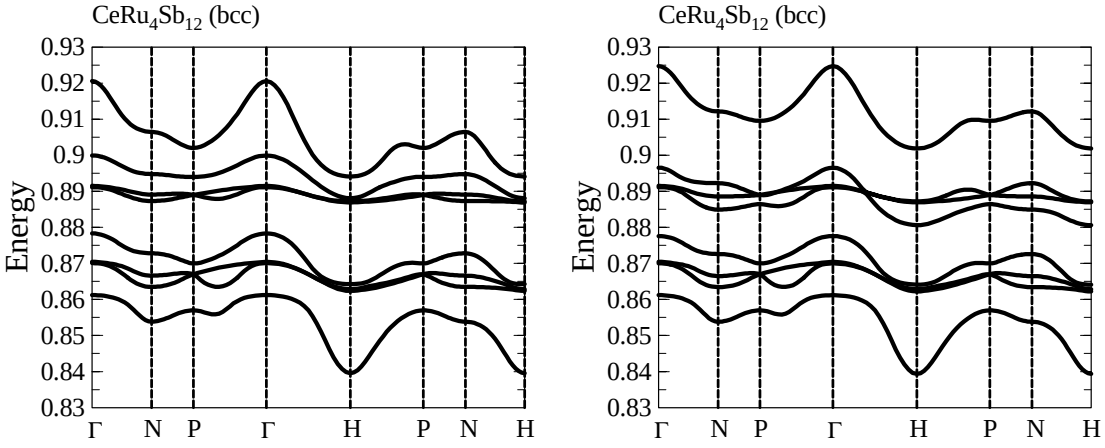

Figure 1: The tight-binding bands for $CeRu_4Sb_{12}$-like model and for (a) $y = 0$ and (b) $y = 2.5 \times 10^{-5}$. $\Gamma_5^{(2)}$, $\Gamma_5^{(1)}$, Γ_{67} for $J = 7/2$, Γ_5, Γ_{67} of $J = 5/2$, and the HOMO band of pnictogen X_{12} clusters, respectively, from top to bottom.

[1] T. Mutou and T. Saso: J. Phys. Soc. Jpn. **73** (2004) 2900.