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Fermi surfaces of $PrOs_4Sb_{12}$ based on the LDA+U method

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Abstract

Fermi surfaces of $PrOs_4Sb_{12}$ are investigated based on the LDA+U method with many U values The $4f^2$ electrons in $PrOs_4Sb_{12}$ are experimentally suggested to be localized, in contrast with other heavy fermion superconductors. This study has revealed that the $4f$ electrons remain localized with small $U = 0.1Ry$, then become itinerant with $U = 0.05Ry$, where the topology of the Fermi surfaces are changed and no longer explains the dHvA measurement.

Key words: $PrOs_4Sb_{12}$, LDA+U method, Fermi surface

The filled skutterudite compounds with a general formula RT_4X_{12} (R=Rare earth, Th and U; T= Fe, Ru and Os; X= P, As and Sb) have recently attracted much attention for the variety of the electrical and magnetic properties. Among them, $PrOs_4Sb_{12}$ has been reported to undergo superconductivity at $T_c = 1.85K$ with the large electronic specifc heat coefficient $\gamma = 350 \sim 700\mathrm{mJ/mol{\cdot}}K^2$[1,2]. Unconventional superconducting properties have been reported from the thermal conductivity[3], the NMR measurement[4] and the μSR measurement[5]. In applied magnetic fields, another ordered phase appears above the upper critical field [6]. The neutron measurement has suggested that quadrupole interactions should play a crucial role in the field induced ordered phase[7].

The measurements of the de Haas-van Alphen (dHvA) effects have revealed that the topology of Fermi surface (FS) of $PrOs_4Sb_{12}$ is very similar to that of the reference compound $LaOs_4Sb_{12}$.[8] It indicates that the $4f^2$ electrons in $PrOs_4Sb_{12}$ are well localized, in contrast with other heavy fermion superconductors. The LDA+U method can treat such localized electrons in a unfilled shell within a band picture. The ground state of $4f^2$ in $PrOs_4Sb_{12}$ suggested to be a singlet and such the localized singlet ground state can be obtained without any symmetry breaking. In fact, the FSs obtained by the LDA+U method with a parameter $U = 0.4Ry$, have explained well the angular dependence of the dHvA experiments .[8] In the bandstructure, $4f^2$ electrons are located below the Fermi level and well localized. Therefore, the density of states at the Fermi level contains only a small amount of f component (a few %), though the measured cyclotron masses are largely enhanced in $PrOs_4Sb_{12}$. Then the question arises how the U value affects the topology of the FSs and the mass enhancement. In this study, the U dependence of the electronic bandstructures have been investigated. Calculations with $U = 0.4Ry, 0.3Ry, 0.2Ry, 0.1Ry, 0.05Ry$ and $0Ry$ (LDA) have been performed self-consistently.

Figure 1 (a) shows the bandstructure in the vicinity of the Fermi level with $U = 0.4Ry$, which is very similar to the case of non f reference $LaOs_4Sb_{12}$.[9] The hole FSs around the N points is observed as the γ branch, and the cyclotron masses are the most largely enhanced.[8] As shown in Fig. 1 (b), the bandstructure near the Fermi level remains unchanged with down to $U = 0.10Ry$. The electronic specific heat coefficient (the density of states at the Fermi level) γ is 43.3 $\mathrm{mJ/mol{\cdot}K^2}$ and the f-component is still less than 10%. As shown in Fig. 2 (a), the main part of the f-

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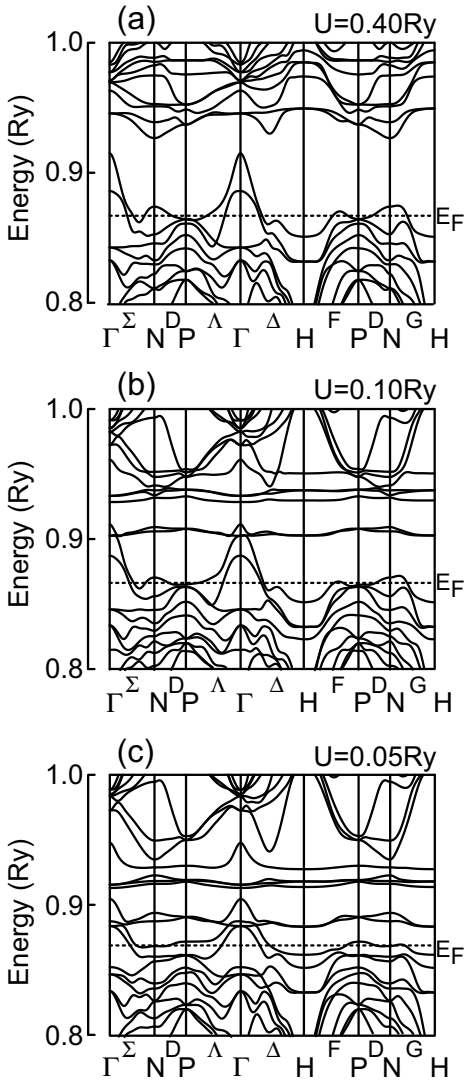

Fig. 1. The LDA+U bandstructures for $PrOs_4Sb_{12}$ with $U = 0.40Ry$ (a), $U = 0.10Ry$ (b) and $U = 0.05Ry$ (c). Note that the topology of FSs are changed between (b) and (c).

components are located well below and above the Fermi level, so the $f$electrons are regarded as still localized.

When U is set as $0.05Ry$, the FSs are topologically changed, *i.e.* the hole FSs around the N points disappear. The f-components are situated on the Fermi level, then affect the FSs (see Fig. 1(c) and Fig. 2 (b)). This corresponds the f itinerant picture. The γ value becomes large as 81.5 mJ/mol·K^2 in which the f-component is about 50%. However, the FSs containing such large f-component could not explain the angular dependence of the dHvA measurements.

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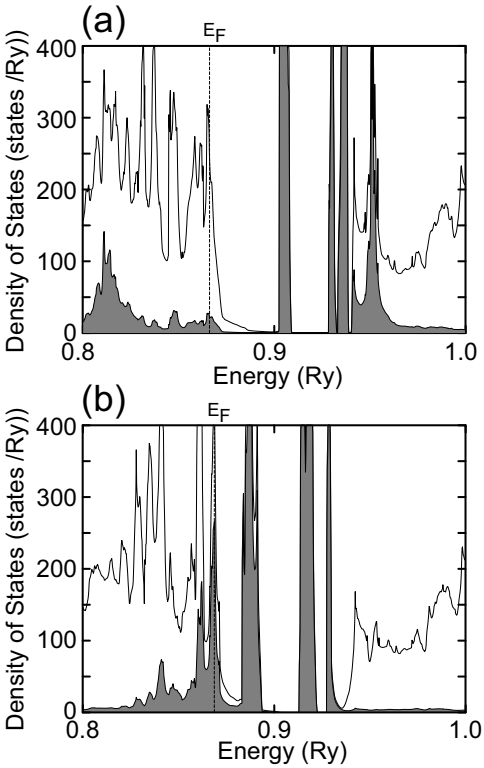

Fig. 2. The LDA+U density of states for $PrOs_4Sb_{12}$ with $U = 0.10Ry$ (a) and $U = 0.05Ry$ (b). f-components are indicated by grey parts.

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