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Fermi Surface of the filled skutterudite $LaOs_4P_{12}$

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Abstract

A good nesting property of the main Fermi surfaces causes the variety of the phase transitions realized in the filled skutterudites. However, no such transitions are reported in $R^{3+}Os_4P_{12}$. The electronic structure and the Fermi surfaces of $LaOs_4P_{12}$ are calculated to discuss the role of the nesting property in the phase transitions realized in the filled skutterudites.

Key words: $LaOs_4P_{12}$, skutterudite, Fermi surface
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A family of skutterudites RT_4X_{12} (R=rare earth etc., T=Fe, Ru, Os, X=P, As, Sb) has attracted much attention for the variety of physical properties, e.g. metal-insulator transitions of $PrRu_4P_{12}$[1] and $SmRu_4P_{12}$[2], heavy fermion behavior of $PrFe_4P_{12}$[3], and heavy fermion superconductivity of $PrOs_4Sb_{12}$[4]. Such the properties are strongly related to the characteristics of the Fermi surfaces provided in the unique crystal structure. Actually a good nesting property of the Fermi surfaces of $R^{3+}Ru_4P_{12}$ and $R^{3+}Fe_4P_{12}$ have been revealed by the bandstructure calculations[5], to cause the phase transitions. Experimentally, the dHvA effect is observed to confirm such Fermi surface properties in $LaFe_4P_{12}$[6] and $LaRu_4P_{12}$[7]. However, no such the phase transition is realized in $R^{3+}Os_4P_{12}$, though the main Fermi surface consists of the P-p molecular orbital[8]. The recent experimental study has revealed that $PrOs_4P_{12}$ shows no phase transition down to 0.1 K[9] and a heavy cyclotron mass is observed in the dHvA effect[10]. In this paper, a bandstructure of $LaOs_4P_{12}$ has been calculated to clarify the Fermi surface property.

The crystal structure of the skutterudites is a unique body centered structure with the space group $Im\bar{3}$ (T_h^5, #204). The lattice constant is reported as 8.0844Å[11], but no parameters of P-position has been reported, then (u, v) =(0.1504, 0.3539) as in $LaFe_4P_{12}$[6] are used in the calculation. The bandstructure calculation has been carried out by using an FLAPW method within the LDA, as was done for $LaFe_4P_{12}$[6]. The spin-orbit interaction is taken into account as a second variational procedure.

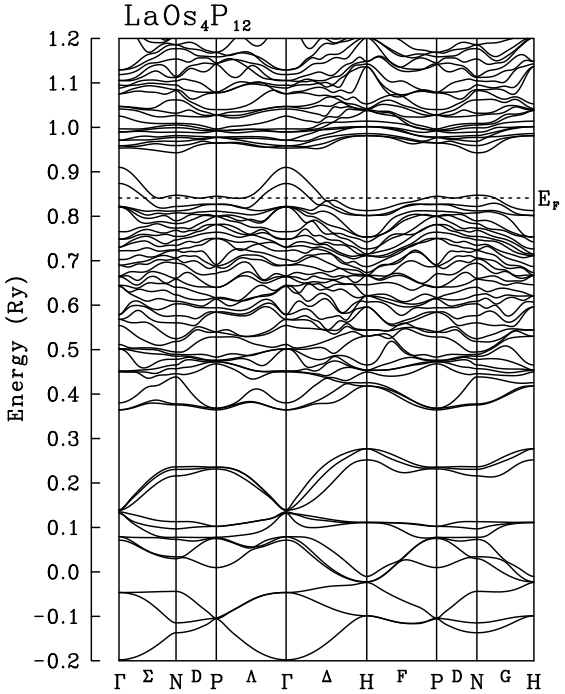

Fig. 1. Eletronic bandstructure of $LaOs_4P_{12}$

Figure 1 shows the calculated bandstructure for $LaOs_4P_{12}$. Two conduction bands (the 47th and 48th) cross the Fermi level. This is similar to that of $LaFe_4P_{12}$[6] and $LaOs_4Sb_{12}$[12]. The lower band, consisting of the Os-$d(a_g)$ band, produces the closed hole Fermi surface, while the

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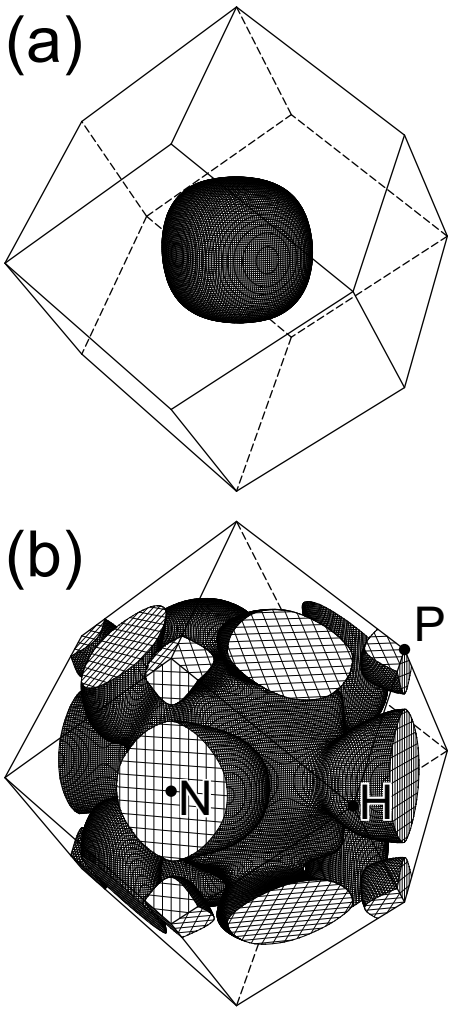

Fig. 2. (a) 47th and (b) 48th Fermi surfaces of $LaOs_4P_{12}$.

upper band, mainly consisting of the P-p electrons, forms a multiply connected Fermi surface, as shown in Fig. 2.

In $LaFe_4P_{12}$, the Fermi surface is connected at the P and the N points, but not at P points in $LaOs_4P_{12}$, as in Fig. 2 (b). In Fig. 2 (b), it is easy to find a small cube centered at the Γ point, which is the Fermi surface with the good nesting property, derived from the a_u orbital.[8] The Fermi surface becomes small in size due to the existence of the 47th ($d(a_g)$) Fermi surface and the other parts around the N and P points in the 48th Fermi surface, so that the nesting vector becomes smaller than $q = (1, 0, 0)$. Such the Fermi surfaces around the N and P points originate in the hybridized band from the Os-d and the P-p band. The populations of some components inside the MT (muffin-tin) spheres are listed in Table 1.

Now let us compare the Fermi surface with that of $LaOs_4Sb_{12}$[12]. The closed surface around the P point does not exist, and the Fermi surface around the N point becomes separated from the surface centered at the Fermi surface, and enlarged to connect each other in $LsOs_4Sb_{12}$[12].

In the case of $PrRu_4P_{12}$, only one Fermi surface appears in the calculation[5], and only one Fermi surface is observed in $LaRu_4P_{12}$[7]. In the case of RRu_4P_{12}, the Ru-d bands

Table 1
The populations of some components inside the MT spheres of the 48th band. The Fermi level is 0.84096 Ry.

	Energy (Ry)	La-f	Os-d	P-p	outside
Γ point	0.9100	0.29	0.00	0.33	0.29
N point	0.8472	0.06	0.20	0.32	0.32
P point	0.8449	0.07	0.03	0.45	0.35
H point	0.8127	0.00	0.52	0.07	0.26

are situated relatively lower so that the T-d P-p hybridized bands are also located below the Fermi level. Therefore the Fermi surface is almost a cube, which volume is just a half of the BZ, then it has a strong nesting property with $q = (1, 0, 0)$. Except $R^{3+}Ru_4P_{12}$, the T-d bands affect the Fermi surface properties in the filled skutterudites. Even though the extra Fermi surface is realized in $LaFe_4P_{12}$, $PrFe_4P_{12}$ undergoes a nonmagnetic phase transition at 6.5 K with $q = (1, 0, 0)$.[3] On the contrary, no phase transition has been reported down to 0.1 K in $PrOs_4P_{12}$[9]. It might be because the nesting vector is too smaller than $q = (1, 0, 0)$.

Obviously any La-compound does not undergo such the phase transition with $q = (1, 0, 0)$. It strongly indicates that the $4f$ electrons might play the role in the transitions, besides the nesting property. The non magnetic ground state separated by 30-50 K from a first excited triplet state is indicated for $PrOs_4P_{12}$[9], while in $PrFe_4P_{12}$ the first excited triplet state is separated by less than only a several degrees[3]. The small crystalline field splitting yields a large number of freedom in f electrons, e.g., higher multipoles, one of which is realized in $PrFe_4P_{12}$[13]. The small crystalline splitting is also necessary to cause the unique phase transitions in the filled skutterudites. The detailed Fermi surface study for $LaOs_4P_{12}$ and $PrOs_4P_{12}$ will be published in a separate paper.

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