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Electronic bandstructure calculations on the filled skutterudites

H. Harima[1] and K. Takegahara[2]

1 - The Institute of Scientific and Industrial Research, Osaka University
Ibaraki, Osaka 567-0047, Japan

2 - Department of Materials Science and Technology, Hirosaki University
Hirosaki, Aomori 036-8561, Japan

Since 1996, we have investigated electronic bandstructures for various filled skutterudite compounds, based on an FLAPW method within the LDA and LDA+U treatment.[1-13]

In cooperating with experimental groups, the Fermi surfaces have been revealed for $LaFe_4P_{12}$ [1,3], $LaRu_4P_{12}$ [10], $LaRu_4Sb_{12}$[14], $LaOs_4Sb_{12}$ [11] and $PrOs_4Sb_{12}$ [7].

The underlying property of the Fermi surface nesting with $\mathbf{q} = (1, 0, 0)$ has been discussed for the structural phase transitions of $PrFe_4P_{12}$ [3] and $PrRu_4P_{12}$ [4,5,8,13]. The nesting Fermi surface originates in the unique P_{12}-p molecular orbital, which symmetry is xyz or a_u in T_h group[13]. This conduction band shows a peak structure in the density of states, indicating instability in the electron system. Actually, bandstructure calculations for the supercell structure for $PrRu_4P_{12}$ [8] have revealed that the small P-displacement could bring the Metal-Insulator (M-I) transition, which is observed around 60 K. However, no distinct reason has been provided for why $LaRu_4P_{12}$ does not show such the M-I transition, though they have very similar Fermi surfaces. The dHvA result for $PrFe_4P_{12}$ has not well explained from the bandstructure calculations, so far, probably due to its unique ground state.

Recently, we have developed our program code to obtain the electric field gradient (EFG) coefficients in general, then the results are compared with the measured NQR frequencies. The quadrupole moments, unfortunately, has not been settled for many nuclei, so the direct comparison could not been performed so far. However, the calculated anisotropic parameter ($\eta = 0.45$) and the direction of the principle axes for $LaOs_4Sb_{12}$ show good agreement with experimental results ($\eta = 0.46$) for $PrOs_4Sb_{12}$.

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