(PS6)

Electronic band structures of the filled skutterudites with ferromagnetic order

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Band structure calculations for the ferromagnetic $EuFe_4P_{12}$, $EuFe_4Sb_{12}$ and $EuRu_4Sb_{12}$ are carried out using the FLAPW method with the LSDA. We get the stable ferromagnetic solution for these compounds. The calculated results for $EuFe_4Sb_{12}$ are shown in Figure 1.

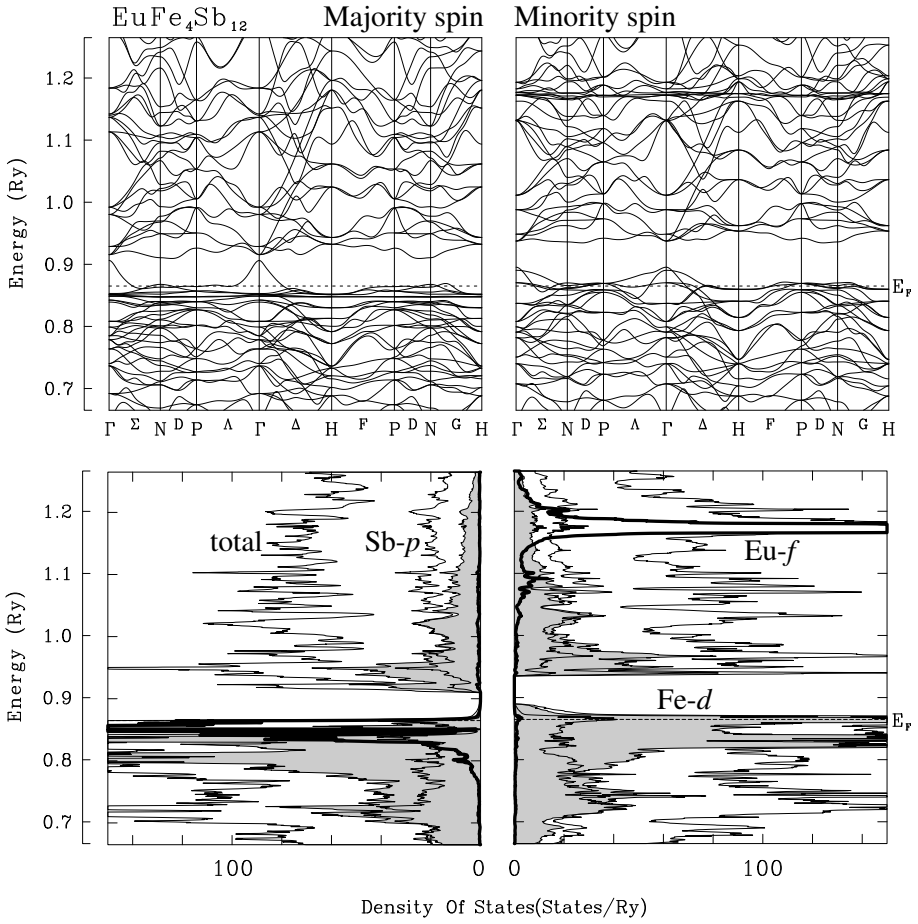

Figure 1: The energy band structures and total and partial DOS of ferromagnetic $EuFe_4Sb_{12}$.

Next we performed the spin-polarized calculations for alkaline earths-based filled skutterudites. The starting charge density was obtained by superposition of self-consistent charge densities for neutral atoms in which the Fe and Ru atoms are in the spin-polarized states; the electron configuration of Fe is $\cdots 3d^5 4s^1$ (majority spin) and $\cdots 3d^1 4s^1$ (minority spin), and Ru is $\cdots 4d^5 5s^{0.5}$ (majority spin) and $\cdots 4d^2 5s^{0.5}$ (minority spin).

For $BaRu_4Sb_{12}$ and $SrRu_4Sb_{12}$, after several steps of the self-consistent iteration processes, the spin polarizations on Ru atom decreased rapidly. Therefore, the ferromagnetic ground state in $BaRu_4Sb_{12}$ and $SrRu_4Sb_{12}$ was considered to be unstable within the LSDA.

For $BaFe_4Sb_{12}$, we get the stable ferromagnetic solution. This is because the Fe $3d$ state has more localized character than the Ru $4d$ state and the Fe $3d$ levels of Fe-Sb skutterudite are the shallowest. We are now calculating the ferromagnetic band structures for $SrFe_4Sb_{12}$ and $CaFe_4Sb_{12}$.