

Band Gap, Electron Localization, and Thermoelectricity in CeRhAs and Related Compounds

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Abstract

We have performed first-principles band structure calculations of orthorhombic ϵ -TiNiSi type CeRhAs and related ternary intermetallic compounds. Results of the calculations predict that the ground state of CeRhAs is insulating with an indirect band gap of 38 meV [1]. On the other hand, the ground state of CeRhSb, CeT₂Sn (T =Ni, Pt) is semimetallic with anisotropic hole and electron pockets. These qualitative properties are in agreement with experimental results of electrical resistivity measurements. The difference in the electronic structure near the E_F originates in hybridization of Ce f orbitals and Rh, Ni, Pt $d - X$ (X =As, Sn, Sb) p anti-bonding orbitals. CeRhAs have less Ce f states in valence states than CeRhSb, CeT₂Sn (T =Ni, Pt). We have calculated electron localization tensor for CeRhAs to investigate hybridization of Ce $4f$ states to valence states. The localization tensor for each direction are comparable magnitude that of Ge $s-p$ electrons. This results are consistent with weak hybridization of localized Ce f states to valence states.

In order to discuss the thermoelectricity, we calculate temperature dependence of Seebeck coefficient $S(T)$ from Boltzmann transport theory with the constant relaxation time. $S(T)$ for both f and non- f electron semiconducting intermetallic compounds are calculated. Then we discussed the role of f -electron states in thermoelectricity.

[1]F. Ishii, Physica B in press.