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First principle study of the electronic structure, Fermi surface, electronic charge density and optical properties of $ThCu_5In$ and $ThCu_5Sn$ single crystals

Abstract

The electronic structure, Fermi surface, electronic charge density and optical properties of $ThCu_5In$ and $ThCu_5Sn$ single crystals are studied. The calculations are based on the full potential-linearized augmented plane wave (FPLAPW) method. The exchange and correlation potential is treated by the local density approximation (LDA) and generalized-gradient approximation (GGA), in addition the Engel–Vosko (EV-GGA) formalism was also applied. The DFT calculations show that these compounds have metallic origin. The contribution of different bands was analyzed from total and partial density of states curves. The values of the density of states at Fermi energy ($N(E_F)$) for $ThCu_5In$ ($ThCu_5Sn$) is 1.75 (1.63) states/eV unit cell. The bare electronic specific heat coefficient (γ) is found to be equal to 0.30 and 0.28 mJ/mol-K^2 for $ThCu_5In$ and $ThCu_5Sn$, respectively. The Fermi surface of $ThCu_5In$/$ThCu_5Sn$ is composed of three/four bands crossing along the R–Γ direction. The bonding features are analyzed by using the electronic charge density contour in the (101) crystallographic plane and it shows the covalent character of Cu–Cu and Sn/In–Cu bonds. The optical properties were also calculated and analyzed.

Keywords; FPLAPW calculation, Electronic structure, Charge density, Optical property, DFT