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Study of electronic structure, charge density, Fermi energy and optic properties of Cs2KTbCl6 and Cs2KEuCl 6

Abstract

Through the assist of the full-potential linear augmented plane wave (FPLAPW) method, the calculations of the electronic band structure, density of states, charge density, Fermi energy and regularity dependent dielectric functions of Cs2KTbCl6 and Cs2KEuCl6 are reported. This study shows that the nature of both these compounds is metallic. The generalized gradient approximations (GGA) exchange correlation potential was applied. The densities of states around Fermi level are frequently subjugated by Eu/Tb-f and DOS below Fermi level are subjugated by Eu/Tb-s/d, Cs-s, Cl-s and K-s/p. The value of the DOS at Fermi level N(EF) is 17.02 and 4.86 (states per unit cell per eV) for Cs2KEuCl6 and Cs2KTbCl6. The bare electronic specific heat coefficient, is found to be 2.95 and 0.84 mJ/mol K2 for Cs 2KEuCl6 and Cs2KTbCl6, respectively. Three bands crossing the Fermi level along the Γ-A direction of Brillion zone of Cs2KTbCl6 compound and one band crossing along the Γ-A direction of Brillion zone of Cs2KEuCl6compounds, to form the Fermi surface. There exists a strong hybridization between Tb/Eu-K-p and Cl-s K-s and at -5.0 and -4.0 eV.

Keywords

DFT; Europium compounds; GGA; Terbium compound