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Electronic band structure and optoelectronic properties of SrCu2X2(X = As, Sb): DFT calculation

Abstract

All-electron-full potential linear-augmented plane wave method with Engel Vosko approximation was used for calculating the electronic structure, Fermi surface, and optical properties of SrCu2X2 (X = As, Sb). The calculated band structure and Fermi surface show that the metallic behavior of SrCu2X2 increases as one move from As to Sb. The calculated partial density of states shows that As-s/p/d, Cu-s/p, and Sr-s/p/d states are forming the Fermi surface for SrCu2As2, whereas Sb-s/p/d, Cu-s/p, and Sr-s/p/d states are forming the Fermi surface for SrCu2Sb2. The calculated densities of states at Fermi level and electronic specific heat are 14.2 (42.57) states/Ryd-cell and 2.60 (7.37) mJ/mol 2 for SrCu2As2 (SrCu 2Sb2). The complex optical dielectric function's dispersion and the related optical properties such as refractive indices, extension coefficient, absorption coefficient, reflectivity, energy loss function, and optical conductivity were calculated and discussed in detail. The optical properties show a considerable anisotropy between the two components.

Keywords

Electronic band structure; Optoelectronic properties; Fermi surface