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Thermoelectric properties, electronic structure and optoelectronic properties of anisotropic $Ba_2Tl_2CuO_6$ single crystal from DFT approach

Abstract

First principle calculation was performed for the electronic structure, electronic charge density, Fermi surface, optical and thermoelectric properties of $Ba_2Tl_2CuO_6$ compound. From the electronic band structure the two overlapping bands and the density of state at Fermi level (29.2 states/Ryd-cell) confirms the superconducting behavior. Colors of the Fermi surface elucidate speed of electrons and strength of the superconductivity as well. The bonding nature was investigated using the calculated charge density contour plot, it shows mixed ionic-covalent nature of Cu3O and Tl3O while Ba3O shows dominant ionic nature with small covalency. The optical properties were calculated and discussed in details. The calculated uniaxial anisotropy value (0.7913) clarifies a considerable anisotropy between two dominant tensor components of dielectric function. Moreover the evaluation of Seebeck coefficient and thermal conductivity conform that the compound is much suitable for thermoelectric applications.

Keywords; Superconductor, Fermi surface, Optical property, Seebeck coefficient