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Electronic structure, Fermi surface and optical properties of metallic compound $Be_8(B_{48})B_2$

Abstract

The band structure, density of states, electronic charge density, Fermi surface and optical properties for $B_8(Be_{48})B_2$ compound has been investigated in the support of density functional theory (DFT). The atomic positions of $B_8(Be_{48})B_2$ compound were optimized by minimization of the forces acting on the atoms using the full potential linear augmented plane wave (FPLAPW) method. We have employed the local density approximation (LDA), generalized gradient approximation (GGA) and Engal-Vosko GGA (EVGGA) to indulgence the exchange correlation potential by solving Kohn–Sham equations. The result shows that the compound is metallic with sturdy hybridization near the Fermi energy level (E_F). The density of states at Fermi energy, $N(E_F)$, is determined by the overlaping between B-p, B-s and Be-s states. This overlaping is strong enough indicating metallic origin with different values of $N(E_F)$. These values are 16.4, 16.27 and 14.89 states/eV, and the corresponding bare linear low-temperature electronic specific heat coefficient (γ) is found to be 2.84, 2.82 and 2.58 mJ/mol K^2 for EVGGA, GGA and LDA respectively. There exists a strong hybridization between B-s and B-p states, also between B-s and Be-p states around the Fermi level. The Fermi surface is composed of three sheets. These sheets consist of set of holes and electrons. The bonding features of the compounds are analyzed using the electronic charge density in the (101 and −101) crystallographic planes and also the analyzing of charge density shows covalent bonding between B and B. The linear optical properties are also deliberated and discussed in particulars.

Keywords; Ceramics, Metals, Electronic structure, Fermi surface, Optical properties