Electronic structure, chemical bonding features, and electron charge density of the double-cubane single crystal $[Sb_7S_8Br_2](AlCl_4)_3$

Abstract

The present calculations were performed using all-electron full potential linearized augmented plane wave method based on the density functional theory. We have optimized the structure of the double-cubane single crystal $[Sb_7S_8Br_2](AlCl_4)_3$, starting with the x-ray diffraction data Zhang, [J. Am. Chem. Soc. 131, 9896 (2009)], by minimization of the forces (1 mRy/au) acting on the atoms, keeping the lattice parameters fixed at the experimental values. Our calculations show that $[Sb_7S_8Br_2](AlCl_4)_3$ possesses a wide indirect energy band gap of about 1.6 eV (2.03 eV) using local density approximation (Engel-Vosko generalized gradient approximation) exchange correlation potentials. To describe the bonding properties we have evaluated the electronic charge space density contour in four planes-namely (001), (110), (100), and (010) which show that this compound possesses a considerable anisotropy. The contour plot shows partial ionic and strong covalent bonding between S-Sb, Al-Cl, S-Br, S-S, Cl-Cl, and Sb-Br atoms.