Electronic structure, chemical bonding features, and electron charge density of the double-cubane single crystal \([\text{Sb}_7\text{S}_8\text{Br}_2] (\text{AlCl}_4)_3\)

**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 \([\text{Sb}_7\text{S}_8\text{Br}_2] (\text{AlCl}_4)_3\), starting with the x-ray diffraction data Zhang, \([\text{J. Am. Chem. Soc.} 131, 9896 (2009)]\), by minimization of the forces \((1 \text{ mRy/au})\) acting on the atoms, keeping the lattice parameters fixed at the experimental values. Our calculations show that \([\text{Sb}_7\text{S}_8\text{Br}_2] (\text{AlCl}_4)_3\) possesses a wide indirect energy band gap of about 1.6 eV \((2.03 \text{ eV})\) 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 \((001), (110), (100), \text{and } (010)\) 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.