Single-crystal oxoborate $(Pb_3O)_2(BO_3)_2WO_4$: Growth and characterization

Abstract

An oxoborate, $(Pb_3O)_2(BO_3)_2WO_4$, has been prepared by solid-state reaction methods below 620°C. Single-crystal XRD analysis shows that it crystallizes in the orthorhombic group Cmcm with a = 18.480(4) , b = 6.3567(13) , c = 11.672(2) , Z = 4. The crystal structure is composed of one-dimensional $1_\infty[Pb_3O]^{4+}$ chains formed by corner-sharing OPb_4 tetrahedra. BO_3 and WO_4 groups are located around the chains to hold them together via PbO bonds. The IR spectra further confirmed the presence of BO_3 groups. Furthermore we have performed theoretical calculations by employing the all-electron full potential linearized augmented plane wave (FP-LAPW) method to solve the Kohn Sham equations. Starting from our XRD data we have optimized the atomic positions by minimizing the forces. These are used to calculate the electronic band structure, the atomic site-decomposed density of states, electron charge density and the chemical bonding features. The calculated electronic band structure and densities of states suggest that this oxoborate possesses a wide energy band gap. The valence band maxima and the conduction band minima are located at Y point in the Brillouin zone resulting in a direct energy band gap of 2.3 eV using the local density approximation and 2.6 eV for the Engel-Vosko generalized gradient approximation. This compares well with our experimentally measured energy band gap of 2.9 eV. From our calculated electron charge density distribution, we obtain an image of the electron clouds that surround the molecules in the unit cell of the crystal. The chemical bonding features were analyzed and the substantial covalent interactions are observed between Pb and O, B and O and W and O atoms