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Structural and Electronic properties of β-In_2X_3 (X = O, S, Se, Te) using *ab initio* calculations[1] S.V. KHARE, S. MARSILLAC, N.S. MANGALE, V. GADE, University of Toledo — Several III-VI body-centered tetragonal layered compounds belonging to space group $I4_1/amd$ have been a subject of interest recently because of their potential applications in high efficiency and environmentally friendly copper-indium-gallium-selenide (CIGS) solar cells and molecules. Here we have studied the structural, energetic, and electronic properties of four compounds β-In_2X_3 (X = O, S, Se, Te), in this space group. Using first principles computations, we have fully determined the lattice constants a and c, as well as 10 internal parameters that define this unique structure of primitive unit cells of 40 atoms. For β-In_2S_3 our computed values are found to be consistent with experimental measurements. The bulk modulus B, local electronic density of states (LDOS), total density of states (DOS), and band gap E_f of these phases have been investigated.

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