# Bismuth Chalcohalides for Optoelectronic Applications

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Bi-based halide perovskites are an interesting class of material because of their rich structural diversity and the ability to exist in a wide range of coordination geometries (from cluster to 1D, 2D, or even 3D) makes them particularly useful for designing novel compounds for optoelectronic applications. Bismuth halides such as $BiI_3$, $A_3Bi_2I_9$ (where A is $Cs^+$ or $CH_3NH_3^+$), chalcogenides ($Bi_2S_3$, $Bi_2Se_3$), and chalcohalides (BiSI, BiSeI, $BiSI_5$,$Bi_2Te_2Br$,$(AlCl_4)_6$), exhibit interesting electrical, magnetic, and optical properties. In this investigation, we report electronic structure, connection to the crystal geometry, density of states and band structure of BiSeI, BiSeBr, $Bi_3Se_4Br$ and BiSI Bismuth chalcohalides as potential optoelectronic materials. All calculations are performed within the framework of density functional theory using the plane-wave pseudopotential method as implemented in the Vienna Ab-initio Simulation Package (VASP). Crystal structures of the bismuth chalcohalides two distinct crystal structures can be identified. BiSeBr, BiSeI, BiSI possess an orthorhombic structure (space group Pmmn,Pnma, Pnma ) and $Bi_3Se_4Br$ possess a monoclinic crystal structure (space group C2/m). According to the band structure analysis BiSeI, BiSeBr, $Bi_3Se_4Br$ and BiSI are found to possess optical band gaps in between 1-1.9 eV. The crystal structure of BiSeBr, and BiSeI has chains of atoms running along the c-axis and have similar electronic properties, including similar optical band gaps of 1.54 eV and 1.56 eV, respectively. The crystal structure of $Bi_3Se_4Br$ shows atomic chains, along the b axis and the calculated band structure is indicates an indirect bandgap (~1.04 eV) with the CBM at k point along the Γ-M direction and VBM along the N-Z direction. BiSI shows well-separated groups of bands and reveal that BiSI crystal has an indirect forbidden gap (1.87eV). The minimum of the conduction band is located at ƛ point and the maximum of the valence band appears nearly midway between the Z and ƛ points. Generally, band gap greater than 1.5 eV can be used for radiation detection applications and further analysis could be carried out to find potential as room-temperature radiation detection materials. According to this study, the band gaps of BiSeI, BiSeBr,$Bi_3Se_4Br$ and BiSI are in the range of band gap required for photovoltaics. Furthermore, other electronic properties, including the effective mass, optical absorption. should be investigated to check the applicability in various optoelectronic devices.

**Keywords**: Band Gap, Optoelectronic, Density of states.