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Full Potential Calculation of Structural and Electronic Properties of Perovskite BiAlO3 and BiGaO3

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Abstract : The first principles within the full potential linearized augmented plane wave (FP-LAPW) method were applied to study the structural and electronic properties of cubic perovskite-type compounds BiAlO3 and BiGaO3. The lattice constant, bulk modulus, its pressure derivative, band structure and density of states were obtained. The results show that BiGaO3 should exhibit higher hardness and stiffness than BiAlO3. The Al–O or Ga–O bonds are typically covalent with a strong hybridization as well as Bi–O ones that have a significant ionic character. Both materials are weakly ionic and exhibit wide and indirect band gaps, which are typical of insulators.

Keywords : DFT, Ab initio, electronic structure, Perovskite structure, ferroelectrics
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