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Direct band gap narrowing and light-harvesting-potential in orthorhombic In-doped-$AlFeO_3$ perovskite: A first principles study

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Abstract:

Enhancing the structural stability of $AlFeO_3$ is relevant since one of the primary reasons for its lack of engineering appeal lies in the fact that the system shows polytypism. This means that the system would have structural transitions in operation. Hence enhancing the stability of a relevant phase becomes central to utilizing the $AlFeO_3$ phase for device applications. Here the crystal structures and ground state properties of $AlFeO_3$ and indium-doped-$AlFeO_3$, i.e $Al_{1-x}In_xFeO_3$ (x=0.25, 0.5, 0.75) are studied using first principles calculations based on density functional theory. Computed ground state properties like equilibrium lattice constants and bulk modulus are in good agreement with the available experimental data. Interestingly In-doped orthorhombic $AlFeO_3$ has higher stability when compared to the parent structure, indicating a simple chemical approach to stabilizing this structure (hence providing a method to avoid the usual polytypism related challenges). Band structures and density of states of these materials phases are reported and analyzed. The experimentally relevant outcomes of this work are: (i) doped compositions when tuned appropriately can show a direct band gap of ~1.12 eV and hence is promising as an active material for a single junction device structure; (ii) in another composition window, a direct band gap of ~2-2.30 eV is readily achievable (which is appropriate for water splitting applications). Hence we show that orthorhombic In-doped $AlFeO_3$ is a stable and a promising non-toxic material for energy harvesting applications.

Keywords: orthorhombic In-doped $AlFeO_3$; light-harvesting; ab-initio electronic structure; optical properties.