Structural, electronic, and thermodynamic properties of post-perovskite NaIrO3

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Abstract

We calculated structural, electronic, and thermodynamic properties of paramagnetic post-perovskite NaIrO3. Our calculations were done in the framework of the density functional theory (DFT), using the full potential-linearized augmented plane wave (FP-LAPW) method, combined with the quasi-harmonic Debye model when studying the thermodynamic properties. We treated the exchange-correlation potential with GGA-PBEsol and GGA-PBEsol + TB-mBJ functionals. The use of the TB-mBJ scheme reduces the valence band dispersion but no band gap appears. The obtained results are reported, discussed, and compared with previous data.

Keywords: Post-perovskite; first-principles calculations; exchange-correlation; structural properties; thermodynamic parameters; electronic structure.