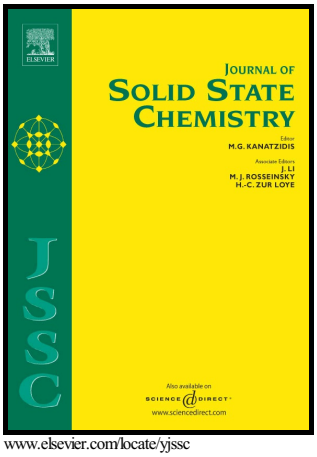

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Ellipsometry; FL-APW; GGA; Band Structure; DOS; Optoelectronic properties;

Abstract

In this study we report results of first-principles density functional calculations using the full-potential linearized augmented plane wave (FP-LAPW) method as implemented in the WIEN2K code. We employed the generalized gradient approximation (GGA) for the exchange-correlation energy to calculate electronic and linear optical properties of the $(C_9H_{19}NH_3)_2PbI_2Br_2$ compound. The linear optical properties, namely, the real $\varepsilon_1(\omega)$ and imaginary $\varepsilon_2(\omega)$ parts of dielectric function, the refractive index $n(\omega)$ and the extinction coefficient $k(\omega)$ are calculated and compared with experimental spectroscopic ellipsometry spectra. The reflectivity $R(\omega)$ and electron energy loss function $L(\omega)$ are calculated too. Our calculations performed for band structure and density of states show that the valence band maximum and conduction band minimum are located at Γ point resulting in a direct band gap of about ($\Gamma_v - \Gamma_c$) of 2.42 eV in good agreement with the experimental data. The investigated compound has a large uniaxial anisotropy of the dielectric function of about 0.0739 and a negative birefringence at zero energy $\Delta n(0) = - 0.11$.

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