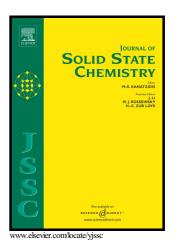
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#### **ACCEPTED MANUSCRIPT**

# Spectroscopic Ellipsometry thin film and First-principles calculations of electronic and linear optical properties of $[(C_9H_{19}NH_3)_2PbI_2Br_2]$ 2D perovskite

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#### Keywords:

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  $\Gamma$  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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