First-Principles Study of the Structural, Optical, and Electronic Properties of the Lead-Halide-Based Organic Perovskites MAPbX3 and FAPbX3 (X= I, Br, Cl)

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Abstract

The electronic properties of MAPbX3 (MA = CH3NH3+) units employing the experimental cell parameters (6.33, 5.95, and 5.66 Å for X = I, Br, and Cl, respectively) and FAPbX3 (FA = CH- (NH2) 2+) units employing the experimental cell parameters (6.36, 5.99, and 5.60 Å for X = I, Br, and Cl, respectively), and the perovskite in the cubic phase have been systematically studied using the first-principles calculations. We have correlated our experimental results with the first-principles theory and provided an insight into important parameters, like lattice constants, the electronic structure, static and high-frequency dielectric constants, reflection coefficient, absorption coefficient, optical conductivity, and the refractive index in these perovskites. Our calculations were performed using the Quantum-ESPRESSO package in the framework of density functional theory (DFT). The projector augmented-wave (PAW) pseudopotentials were used within the energy cutoff of 408 eV for the plane-wave basis functions. For the exchange-correlation functional, the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) was used to relax the structural parameters. We substituted I- to Br- to Cl- in order to tune the bandgap from 1.6 eV to 2.4 eV to 3.2 eV in these materials. Electronic structure calculations reveal that electronic properties are mainly governed by Pb 6p and halide p orbitals. spin-orbit coupling (SOC) is included in all the calculations. All calculations were reported to be in agreement with the experimental data.

Keywords: halide organic perovskites (HOP), dielectric function, absorption, DOS, band structure, solar cell, LED

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