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Optimized opto-electronic and mechanical properties of orthorhombic methylamunium lead halides (MAPbX 3) (X = I, Br and Cl) for photovoltaic applications

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Abstract
Organometallic halide perovskites (OMHPs) are absorbent materials, and can thus be employed in solar cells with power conversion efficiency (PEC) of 22% or higher. Using calculations, this work confirms earlier experimental findings and determines optimal properties to achieve maximum conversion efficiency for OMHPs. Values of energy band gap, density of states, absorption coefficient, refractive index, dielectric constant and elastic constants of orthorhombic methylamunium lead halides (MAPbX 3) (X = I, Br and Cl) family are all calculated using Density Functional Theory (DFT) method with generalized gradient approximation (GGA). The stiffness of (MAPbX 3) (X = I, Br and Cl) is investigated by calculating Young's moduli E constants. Among the series, MAPbI 3 is the stiffest material with E x = 57.24 GPa. The perovskite family members are characterized by their energy band gap variation as: E g MAPbI3, MAPbBr3, MAPbCl3 = 1.626, 2.207 and 2.748 eV, respectively. They also exhibit a remarkable absorption coefficient (α MAPbX3 = 10 5 cm −1) over a wide energy range particularly the visible spectrum [1.65–3.26 eV: 380–750 nm]. The anisotropy of optical properties (MAPbX 3) (X = I, Br) is proven in the near and middle ultraviolet [3.1–5 eV] energy band. © 2019

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Band gap tuning; DFT; Optical absorption; Perovskites; Stiffness

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