عنوان مقاله:

Investigation of Optoelectronics, Thermoelectric, Structural and Photovoltaic Properties of CH۳NH۳SnBr۳ Lead-Free Organic Perovskites

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خلاصه مقاله:

To develop the lead-free organic perovskites, the crystal CH۳NH۳SnBr۳ was selected for their computational exploration which has a vast functional application in optoelectronic area as functional materials.First of all, the electronics band structures, the total density of state, the partial density of state and optical properties were investigated by DFT functional for CH۳NH۳SnBr۳. In general, the band gap of CH۳NH۳SnBr۳was calculated at ۱.۴۲۱ eV by Generalized Gradient Approximation (GGA) with Perdew Burke Ernzerhof (PBE) functional, and the energy gap and open circuit voltage was evaluated. The density of states (DOS) and partial density of states (PDOS) were evaluated to show that how each atom can be contributed to their electronic structure. The optical properties, for instance absorption, reflection, refractive index, conductivity, dielectric function, and loss function were estimated.Further, Sn atom was substituted to design the lead-free molecule, CH۳NH۳SnBr۳ that passed good optoelectronic and optical properties. It can be concluded that Sn atoms containing organic crystal, CH۳NH۳SnBr۳, show narrow band gap in comparison to lead or other heavy metals containing crystals although Sn is smaller in atomic size than Pd atom.

کلمات کلیدی:

Band gap, DoS, PDOS, optoelectronics and organic perovskites