

ABSTRACT

This study investigates the structural and electronic properties of Bi-doped CsSnBr₃ using density functional theory within the generalized gradient Perdew–Burke–Ernzerhof (GGA-PBE) approximation with ultrasoft pseudopotentials (USPP), considering doping concentrations of 12.5, 25.0%, 37.5%, and 50.0%. The results show the incorporation of Bi induces charge redistribution, which modulates the local bonding environment and causes variations in the bond lengths Sn–Br and Bi–Br. Bi substitution causes to a non-monotonic decrease in the energy band gap, decreasing from 0.55 eV in the pristine system to 0.32, 0.11, 0.23, and 0.21 eV at 12.5%, 25.0%, 37.5%, and 50.0% doping, respectively. Band gap analysis shows that the Fermi level is shifted above the conduction band minimum, indicating degenerative n-type semi conductor behavior caused by donor-like states introduced by Bi substitution. The density of states results show that the Bi 6p state contributes near the conduction band, modifying the band gap and reducing the excitation energy. The optical properties are strongly influenced by Bi doping. The dielectric function exhibits metal-like characteristics, as indicated by the negative real part and the finite imaginary part at low photon energies, associated with the presence of free carriers. This results in enhanced low-energy absorption and shifts in optical transitions due to band gap narrowing and band filling. Reflectivity increases at low energies, with a blue shift and reduced maximum in the visible range. The loss function reveals low-energy free carrier features and high-energy interband transitions. Overall, Bi doping effectively tunes the electronic and optical properties of CsSnBr₃, highlighting its potential for optoelectronic applications, particularly infrared and photodetection technologies.

Keywords : CsSnBr₃ Perovskite, Bi Doping, Optoelektronik, Density Functional Theory

Pembimbing I

Pembimbing II

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