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Density Functional Theory Study of Zn Doped CsPbI3 Perovskite for Photovoltaic and Optoelectronic Applications

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The structural, electronic, and optical properties of the undoped and transition metal Zn doped CsPbI3 were investigated using first-principles calculations within the framework of spin polarised density functional theory implemented in VASP code. The calculations are performed using the local spin density approximation GGA+U method in order to correct the strong Coulomb interactions of 3d electrons. The substitution of Pb atom with the Zn atom reduces the bond length and lattice constants of CsPbI3 due to Zn atom having a smaller ionic radius compared to the Pb atom. The calculated band gap of undoped CsPbI3 is a direct band of 1.488 eV and of Zn doped is an indirect band gap of 0.717 eV. radiation indicate that the materials could be good candidates for solar cell applications. The study of the mechanical properties demonstrates that Zn doped material is mechanically stable and ductile nature as the undoped CsPbI3 compound.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

PhD

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