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Electronic and Optical Properties of Lead-free Hybrid Perovskite CH₃NH₃SnI₃ from first principles calculations

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Organic-inorganic halide perovskites have recently emerged as promising candidates for low cost, high-efficiency solar cells. In this work, the electronic and optical properties of the lead-free hybrid halide perovskite CH₃NH₃S as a solar cell absorber has been investigated using first-principles density functional theory calculations and many body perturbation theory. Our calculated electronic band gaps are 0.77, 1.23 and 1.40 eV using the Perdew, Burke and Ernzerhof, the modified Becke-Johnson and the hybrid functional HSE06, respectively. CH₃NH₃SnI₃ has been reported to have a band gap of 1.21 and 1.35 eV depending on the preparation method. Our calculated band gap using the modified Becke-Johnson and hybrid functional HSE06 agree well with experimental results. The investigated compound (CH₃NH₃SnI₃) is found to be a direct band gap semiconductor with fundamental band gap (1.44 eV). In order to obtain optical spectra, we carried out Bethe-Salpeter equation calculations on top of non-self-consistent G₀W₀ calculations. Our calculated band gap using Bethe-Salpeter equation calculations is 1.22 eV, within the experimentally reported range, confirming that CH₃NH₃SnI₃ has potential as a solar cell absorber.

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