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CsGeI 3 , a Ge-based perovskite halide with Photovoltaic capabilities

Photovoltaic solar cells (PSCs) have undergone a metamorphosis by adopting the halide perovskites with a chemical formula of ABX3. The ABX3 PSCs have arose a lot of research interests due to their high power conversion efficiency (PCE) of ≈22%. Traditionally for a long time, PSCs were based on hybrid organic-inorganic iodide CH3NH3PbI3, but due to the toxic Pb and its chemical instability, it posed both environmental and large-scale commercialization threats. To address these challenges, researchers opted for composition tuning using nontoxic Sn2+ or Ge2+ for Pb2+ and inorganic Cs+ or Rb+ for the organic part in CH3NH3PbI3. Unfortunately, Sn-based perovskite photoabsorbers have been associated with coarse efficiency due to the large mismatch of band alignment between them and charge carrier conductors. The other detriment of the Sn-based perovskites is the susceptibility of Sn oxidation from +2 to +4 state upon exposure to air and this has slowed research efforts in Sn-based PSCs. It is for the above-mentioned reasons that Ge-based inorganic perovskites, have stood out as the best alternatives for the Pb free and long term PSCs. It has been reported experimentally that CsGeI3 stabilizes in the rhombohedral phase with R3m space group at room temperature and theorists have equally tested its structure formidably by analyzing its Goldschmidt tolerance factor. Here in, we will perform a theoretical investigation based on state-of-the-art density functional theory (DFT) as implemented in the quantum ESPRESSO computer code, to get a comprehensive understanding of CsGeI3 for solar cell applications. The structural and optoelectronic properties of inorganic CsGeI 3 halide perovskite will be calculated by the use of PBEsol functional without SOC effect. This project will guide experimentalist in designing novel PSCs for future technologies. We also recommend other studies to be conducted when Cs is replaced with Rb so as to get better PSCs.

Keywords

PSCs; CsGeI 3 ; Density Functional Theory; opto-electronic

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