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# Computation of Electronic and Structural Properties of Tin halide Perovskites for Photovoltaic Application by first principles

Computation of Electronic and Structural Properties of Tin halide Perovskites for Photovoltaic Application by first principles

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Abstract
Lead free perovskites have gained much research interest due to their environmental friendliness. Tin being non toxic has become a viable alternative perovskite and also it has been proven to have lower band gap and wide absorption range compared with the lead counterparts. However the oxidation state of 2+ is still a major setback to achieving higher efficiencies. In this theoretical study the orthorhombic phases of Dimethyl ammonium tin tri-iodide (DASnI3) and Methyl ammonium tin tri-iodide (MASnI3) were studied by first principle calculations based on Density functional theory (DFT) . It was found that a direct band gap was at gamma symmetry points using PBE exchange correlation. Based on comparison with other theoretical and experimental values, the orthorhombic phase of DASnI3 was more stable with the volume of 27.00 a.u.^3 at 544 kbar. It was found that DASnI3 can be more suitable for photovoltaic application compared to the other tin halide perovskites due to its stability.
Key words: first principles, perovskites

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