

**COMPUTATIONAL STUDY ON LEAD ALTERNATIVE  
PEROVSKITES FOR PEROVSKITE SOLAR CELLS**

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Degree of Master of Science

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Sri Lanka

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Thesis submitted in partial fulfillment of the requirements for the degree

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## **DECLARATION**

I declare that this is my own work and this thesis does not incorporate without acknowledgement any material previously submitted for a degree or diploma in any other University or institute of higher learning and to the best of my knowledge and belief it does not contain any material previously published or written by another person except where the acknowledgement is made in the text.

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## ABSTRACT

Hybrid organic-inorganic metal halide based perovskite solar cells (PSCs) lie at the heart of the emerging technologies of the solar cells due to their ability to increase the cell efficiencies dramatically over the last decade.  $\text{CH}_3\text{NH}_3\text{PbI}_3$  based PSCs show the highest performances; still, the toxicity of Pb has been the limiting factor for the commercialization of organic lead iodide based solar cells. This thesis discusses about the variations of properties in terms of electronic and dielectric properties due to the substitution of Sn and Bi in place of Pb. A systematic study of ab-initio calculation on the electronic properties of  $\text{CH}_3\text{NH}_3\text{PbI}_3$ ,  $\text{CH}_3\text{NH}_3\text{SnI}_3$ , and  $\text{CH}_3\text{NH}_3\text{BiI}_3$  was performed. The results of the calculated band structures and the density of states of investigated materials reveal that  $\text{CH}_3\text{NH}_3\text{PbI}_3$  exhibits an energy band gap, effective masses of charge carriers, and available density of states in favorable values for high performance solar cells than those of  $\text{CH}_3\text{NH}_3\text{SnI}_3$  and  $\text{CH}_3\text{NH}_3\text{BiI}_3$ .  $\text{CH}_3\text{NH}_3\text{PbI}_3$  also consists of high dielectric capacity and better energy storage ability than  $\text{CH}_3\text{NH}_3\text{SnI}_3$  and  $\text{CH}_3\text{NH}_3\text{BiI}_3$ . Above mentioned facts are the main reasons behind low-performance of Pb-free PSCs and it is paramount important to engineer the band gaps of those perovskites to obtain high performances.

Keywords: perovskite, efficiency, ab-initio, band gap, mobility, absorption coefficient

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