COMPUTATIONAL STUDY ON LEAD ALTERNATIVE PEROVSKITES FOR PEROVSKITE SOLAR CELLS

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Degree of Master of Science

Department of Materials Science and Engineering

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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

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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. $CH_3NH_3PbI_3$ 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. 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 $CH_3NH_3PbI_3$, $CH_3NH_3SnI_3$, and $CH_3NH_3BiI_3$ was performed. The results of the calculated band structures and the density of states of investigated materials reveal that $CH_3NH_3PbI_3$ exhibits an energy band gap, effective masses of charge carries, and available density of states in favorable values for high performance solar cells than those of $CH_3NH_3SnI_3$ and $CH_3NH_3BiI_3$. $CH_3NH_3PbI_3$ also consist of high dielectric capacity and better energy storage ability than $CH_3NH_3SnI_3$ and $CH_3NH_3BiI_3$. 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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TABLE OF CONTENT

LIST OF FIGURES

LIST OF TABLES