## Abstract

A decade of extensive research has been conducted to enhance the power conversion efficiency (PCE) of silicon (Si) solar cells and to cut their prices short. But still, the fabrication of Si solar cells are costly. So, to reduce the fabrication cost of the solar cell search for alternate earth abundant and non-toxic absorber materials is thriving. Among different absorber materials tin sulfide (SnS) is found to be a suitable candidate for the non-organic solar cell with a band gap of 1.3 eV. But the PCE achieved for SnS is 4.6% that is far less from the PCE of (Si), whereas among other organic non-organic solar cells like methylammonium lead halide perovskite ($MAPbI_3$) is proven to be a suitable candidate with PCE reaching to a value of 23%. The problem with the commercialization of $MAPbI_3$ is due to the toxic nature of lead (Pb). So, in dealing with these issues of solar cell numerical analysis can play a key role as numerical analysis allows flexibility in the design of realistic problem and experimentation with different hypotheses can easily be performed. Complete set of device characteristic can often be easily generated by consuming less amount of time and effort. Because of this reason numerical analysis was used to revisit solar cells design parameters and the effect of solar cell physical parameters on solar cell performance. There are various simulation software's available that are used for solar cell numerical analysis. Here in this work, we used Solar cell capacitance simulator (SCAPS) software, it is freely available and is most popular among the research community. To achieve effective design for efficient solar cell a numerical guide was proposed based on which PCE of an experimental designed solar cell can be enhanced. This was done by reproducing results for the experimentally designed solar cell in SCAPS environment with structure $p - SnS/n - CdS$ having a conversion efficiency of 1.5%. After reproduction of experimental results device performance was optimized by varying thickness of (absorber layer, buffer layer), minority carrier lifetime, doping concentration (absorber, buffer), and adding window layer. By stepwise optimization of device parameters, PCE of an experimental designed solar cell in SCAPS with architecture $p - SnS/n - CdS/n - ZnO$ was reached to a value of 14.01%. From the analysis, it was found that PCE of a solar cell is highly depended upon doping concentration of the absorber layer, the thickness of the absorber layer and interface defects. Based on the results evaluated an analysis was performed for tin based organic non-organic methylammonium tin halide perovskite solar cell ($MASnI_3$) to find the effect of interface recombination on solar cell performance and how it can be governed. The reason for this transition from

SnS to $MASnI_3$ was because $MASnI_3$ can be fabricated simply by spin-coating methylammonium iodide (MAI) over SnS layer. To perform this task analysis was performed for the selection of suitable buffer layer for Pb free methylammonium tin halide perovskite solar cell ($MASnI_3$) and it was found that PCE of the solar cell is also depended upon band alignment between absorber and buffer layer. Based on the results a new structure was proposed for Pb free perovskite solar cell (Back contact/$MASnBr_3$/ $MASnI_3$/CdZnS/FTO) with PCE of 18.71% for absorber thickness of 500 nm and acceptor doping concentration of $1x10^{16}$ $cm^3$. The results achieved in this thesis will provide an imperative guideline for researchers to design efficient solar cells.