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IMPROVING THE EFFICIENCY OF LEAD-FREE NON-TOXIC RUBIDIUM GERMANIUM IODIDE PEROVSKITE SOLAR CELL USING A MOLYBDENUM DISULFIDE INTERFACE LAYER: A SCAPS 1D SIMULATION STUDY

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ABSTRACT

Considering the rising demand for Perovskite solar cells (PSCs) owing to their performance and cost, resolving problems such as interface hysteresis and instability resulting from trap states is essential to PSC economic sustainability. Passivation techniques have being actively developed by researchers to address these issues. In this work, we examine the effects of adding a MoS_2 interface layer to the structure of a perovskite solar cell. Our study concentrates on important performance parameters, with and without the MoS_2 interface layer, such as power conversion efficiency (PCE), fill factor (FF), short circuit current (J_{sc}), and open circuit voltage (V_{oc}). Extensive simulations demonstrate our results' notable enhancements. More specifically, the PCE of the $RbGeI_3$ based PSC increases from 15.63% to 17.20% with the inclusion of the MoS_2 interface layer. Moreover, our investigation shows improvements in J_{sc} and FF. By offering a clearer knowledge of how interface layers, such MoS_2, might be used to enhance PSC performance, this work fills a significant research need. We provide light on the potential of MoS_2, clarify the mechanisms underlying these improvements, and provide insights into how these tactics could speed the development and improve the efficiency of Perovskite solar cells.

Keywords: SCAPS 1D; Efficiency; MoS_2; Interface Layer; Perovskite Solar Cell.

I. INTRODUCTION

The organic hybrid Perovskite solar cell (PSC) and inorganic hybrid PSC are the categories of third-generation photovoltaic cells that showed potential. Because they are less expensive and have an easier production process than standard silicon photovoltaic cells, these cells are expected to be a good substitute [1]. X-ray diffraction and Raman spectroscopy were used in a number of studies to examine the temperature behavior of $RbGeI_3$ [2]. $RbGeI_3$ thermoelectric, optoelectronic, thermodynamic, structural, and mechanical properties were evaluated using a variety of exchange-correlation functions as well as another study examined the structural, magnetic, and electrical properties of cubic $RbGeI_3$ and $RbDyO_3$ perovskites [3, 4]. Motivated by the discovery of graphene, researchers are investigating 2D materials like WS_2 and MoS_2 for their superior solar cell capabilities [5]. To increase the stability and efficiency of perovskite solar cells (PSCs), MoS_2 was used as an interface between the active layer additive and the Hole transport layer (HTL) / CH3NH3PbI3 [6]. The present paper uses SCAPS 1D to assess the photovoltaic efficiency of $RbGeI_3$. While the electron transport layer (ETL) employs titanium dioxide (TiO_2), the hole transport layer (HTL) uses Spiro-OMeTAD. There are going to be two sections to the simulations. Initially, we model the Photovoltaic Cell of PSC structures in the absence of an interface layer (IL). This will enable comparisons with solar energy. The effect of adding a MoS_2 passivation layer between the absorber and the hole transport layer (HTL) on device performance will then be investigated.

II. METHODOLOGY

Computational modeling methods for studying solar cell performance include SILVACO, COMSOL, SETFOS, ATLAS, and SCAPS. SCAPS-1D versions 3.3.10 was employed in this investigation because of its controllability and ease of use. SCAPS may additionally imitate lit and illuminated cells and build a seven-layer hetero structure cell. The Solar Cell Capacitance Simulator was created at Ghent University in Belgium. To analyze solar cells, this application calculates power conversion efficiency (PCE), fill factor (FF), open circuit voltage (V_{oc}), short circuit current (J_{sc}), the Current-Voltage (IV) Curve.

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III. MODELING AND ANALYSIS

First, we modeled a p-i-n solar cell in which light enters the Electron Transport Layer (ETL) and travels toward the absorber layer, where it splits into electron-hole pairs. We found that hole transport and power conversion efficiency (PCE) were limited in the absence of an interface layer among the absorber layer as well as the HTL. We obtained the material parameters for our simulations from the available literature [7, 8]. We did additional simulations using material values from the literature and added an interface layer between the absorber layer and the HTL to increase performance. The efficiency of these design modifications was validated by the considerable improvement in PCE.

Table 1. PSC Parameters Used in SCAPS 1D

Parameters	TiO_2	$RbGeI_3$	MoS_2	Spiro-OMeTAD
Thickness (nm)	150	400	50	150
Bandgap (eV)	3.2	1.310	1.290	3.0
Electron affinity (eV)	4.00	3.9	4.2	2.2
Dielectric permittivity (relative)	10	23.00	4.0	3.0
CB effective density of states	$2x10^{18}$	$1.4x10^{19}$	$7.5x10^{17}$	$2.2x10^{18}$
VB effective density of states	$1.8x10^{19}$	$2.8x10^{19}$	$1.8x10^{18}$	$1.8x10^{9}$
Electron mobility	$2x10^{1}$	$2.8x10^{1}$	$1x10^{2}$	$2x10^{-4}$
Hole mobility	$1x10^{1}$	$2.7x10^{1}$	$1.5x10^{2}$	$2x10^{-4}$
Shallow uniform donor density	$1x10^{17}$	$1x10^{9}$	-	-
Shallow uniform acceptor density	-	$1x10^{9}$	$1x10^{21}$	$1x10^{17}$
Total Defect Density	$1x10^{15}$	$1 x10^{15}$	$1x10^{15}$	$1x10^{15}$

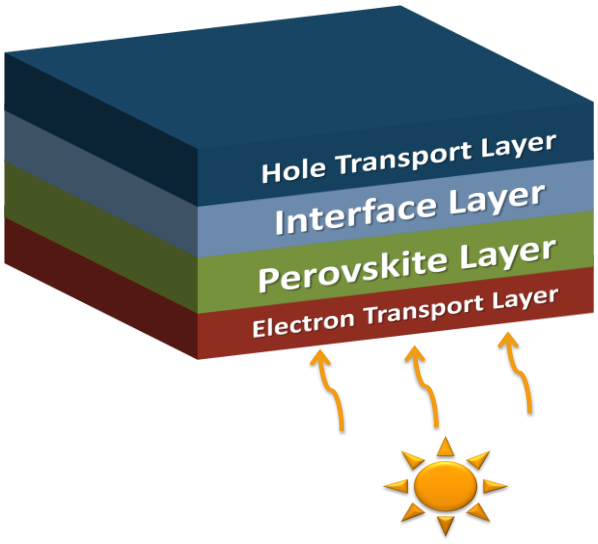

Figure 1: Perovskite solar cell with interface layer

IV. RESULTS AND DISCUSSION

Key photovoltaic parameters, such as the open circuit voltage (0.8V) and short-circuit current (30.7 and 31.6 mA/cm^2), fill factor (FF) (62.58% to 66.30%), and power conversion efficiency (PCE) (15.63% to 17.20%), significantly improved with the introduction of the MoS_2 IL. We were able to analyze the processes underlying

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these improvements using SCAPS 1D simulations. These included the favorable energy level alignment between MoS_2 and $RbGeI_3$ for better charge separation and extraction, as well as the facilitation of efficient charge transport due to MoS_2's high carrier mobility, which decreased recombination losses.

Table 2. Performance of $RbGeI_3$ Based PSC with & without MoS2 as interface layer

Structure	V_{oc}	J_{sc}	FF	Efficiency
$TiO_2/RbGeI_3/Spiro\text{-}OMeTAD$	0.8 V	30.7 mA/cm²	62.58 %	15.63%
$TiO_2/RbGeI_3/MoS_2/Spiro\ OMeTAD$	0.82 V	31.6 mA/cm²	66.30 %	17.20%

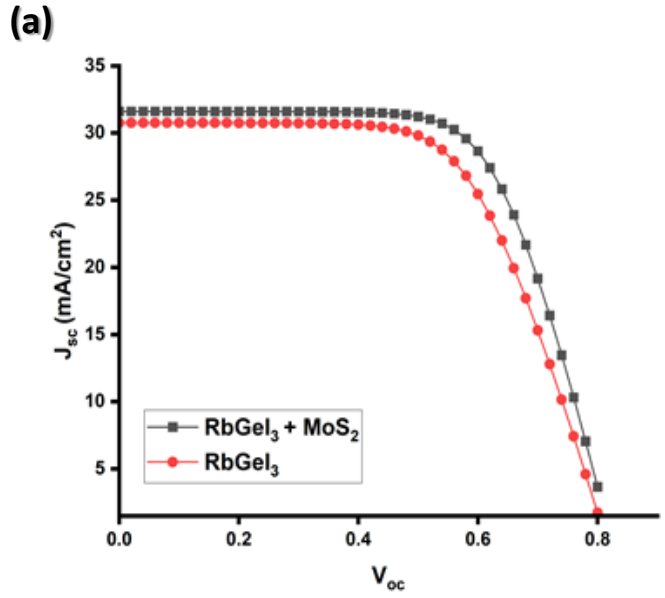

Figure 2: IV Curve of $RbGeI_3$ PSC With and Without MoS_2 Interface Layer.

V. CONCLUSION

In conclusion, this work explores the photovoltaic capabilities of $RbGeI_3$ using SCAPS-1D simulations. Spiro-OMeTAD and titanium dioxides (TiO_2) were used as HTL and ETL, respectively. The performance of the cell is improved by adding a 50 nm MoS_2 layer as an interface layer (IL) between the absorbers in addition to HTL. Based on a comparative analysis of the data, it can be concluded that the MoS_2 interface layer (IL) positively impacts the efficiency of PSCs using $RbGeI_3$ absorber material. Using the MoS_2 layer, $RbGeI_3$ also showed improved performance. The PCE increased from 15.63% to the 17.20%, the fill factor (FF) increased from 62.58% to 66.30%, and the J_{sc} increased from 30.7 mA/cm_2 through 31.6 mA/cm². Perovskite solar cell research in the decades to come should consider many trends and methodologies. First, more investigation into advanced interface materials other than MoS_2 might lead to better device efficiency. For these materials to be economically viable, scalable manufacturing techniques that maintain their quality throughout mass production must be developed. Research on PSC stability and hysteresis issues should continue with the goal to support PSC use on a broader scale. The following studies would need to concentrate on examining novel manufacturing methods and materials that exhibit enhanced environmental sustainability. By addressing these problems and trends, researchers may contribute to the continued success and advancement of perovskite solar cell technology in the field of renewable energy. This work provides valuable insights for the construction and improvement of PSC between absorbers, highlighting the necessity of employing a suitable passivation layer, like MoS_2, to guarantee optimal device performance.

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