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Numerical Study of lead-free halide perovskites solar cells using Efficient materials as electron transport materials

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Abstract

This work presents a comprehensive theoretical analysis aimed at finding the elements that impede the efficiency of KGeCl3 solar cells. The aim of our investigation is to examine the impact of various characteristics to enhance its performance. The improved design exceeds the baseline, attaining a JSC of 37.08 mA/cm², Voc of 0.77 V, and FF of 60.80%, therefore indicating the possibility to reach an efficiency of up to 17.57% by the strategic optimization of 2D materials as the electron transport layer (ETL). The suggested analysis facilitates the identification of relevant degradation components and creates a basis for further design optimization. showcasing the effectiveness of our approach, the findings from this study not only highlight the critical factors affecting 2D perovskite solar cell performance but also provide a foundation for future research and optimization efforts.

Keywords: 2D materials; Solar cells; Simulation; optimization

1. Introduction

Two-dimensional materials have emerged as a prospective frontier in solar cell technology, providing distinctive benefits such as customizable optoelectronic properties and enhanced stability[1-4] However, despite their potential, 2D materials solar cells face several challenges that impact their overall efficiency [5]. Addressing these challenges requires a detailed understanding of how various factors influence the performance of these cells. The efficiency of KGeCl3 perovskite solar cells is influenced by a complex interplay of parameters, including material composition, layer thickness, and fabrication techniques [6]. These factors collectively affect key performance indicators such as short-circuit current density (JSC), open-circuit voltage (Voc), and fill factor (FF). Understanding and optimizing these parameters is essential for enhancing the overall efficiency of the solar cells.This paper presents a comprehensive theoretical analysis aimed at identifying the factors that limit the efficiency of 2D perovskite solar cells. Our approach involves a detailed examination of how different design parameters affect cell performance and the development of optimization strategies to improve efficiency. Through this analysis, we demonstrate that strategic adjustments to the properties of 2D materials can lead to significant improvements, achieving a JSC of 37.57% mA/cm², Voc of 0.77 V, and FF of 60.80%. This optimization results in a potential efficiency of up to 17,57%, showcasing the effectiveness of our approach.

2. Device structure

In our study we utilized a IZO/ TMCs/KGeCI3/Cu2O thin film solar cell configuration, where IZO as the transparent oxide layer, KGeCI3 acted as the absorber layer, MoS2 as the emitter, and Cu2O as hole transport layer,were set at 0.2 µm, 0.5 µm, 0.02 µm and 0.02 µm, respectively.as represente in Figure1. to verify the precision of our proposed model using scaps 1D simulation, The material parameters for modeling were meticulously chosen based on existing data from the literature based on experimental and DFT calculations, as illustrated in Table 1.

3. Modeling framework

SCAPS-1D is a sophisticated simulation tool designed to provide precise insights into the performance of semiconductor devices. It carefully incorporates a range of parameters including defect density, layer thicknesses, carrier concentrations, metal work functions, and the properties of the back hole transport layer (HTL). By solving the fundamental governing equations—such as the Poisson equation and the continuity equations for electrons and holes—SCAPS-1D accurately models the complex behavior of semiconductor structures, as detailed in Eqs (1)-(3). This advanced software is crucial for analyzing and optimizing the performance of our solar cell architecture [11].

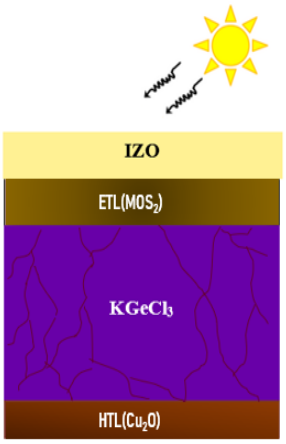

Figure 1. KGeCl3 perovskite solar cell structure

	TCO	ETL	PAL	HTL
Parameters (units)	IZO	MoS2	KGeCl3	Cu2O
Thickness (µm)	0.02	0.02	0.5	0.2
Bandgap (eV)	3.5	1.29	1.1	2
Electron affinity (eV)	4.5	4.2	4	3.8
Dielectric permittivity (relative)	10	4	23.01	10
Effective densityof states (cm-3)CB	$1*10^{19}$	2.2*1018	$6.81*10^{18}$	$3*10^{18}$
effective density of states (cm-3)CV	$1*10^{19}$	$2.2*10^{18}$	$3.45*10^{18}$	$3*10^{19}$
Electron mobility (cm^2/Vs)	10-2	50	92.92	$3.7*10^2$
Hole mobility (cm^2/Vs)	10-3	30	68.59	10^7
Acceptor concentration, NA(cm-3)	0	0	10^{15}	10^{17}
Donor concentration, ND(cm-3)	$1*10^{18}$	$1*10^{18}$	109	0

Table 1. Input parameters values [7-10]

$$\frac{\partial}{\partial x}\left(\varepsilon_0 \varepsilon_R \frac{\delta \psi}{\delta x}\right) = -q\left(p - n + N_d^+ - N_A^- + \frac{\rho_{def}}{q}\right) \quad (1)$$

$$-\frac{\partial J_n}{\partial x} - R_n + G = \frac{\partial n}{\partial t} \quad (2)$$

$$-\frac{\partial J_p}{\partial x} - R_p + G = \frac{\partial p}{\partial t} \quad (3)$$

In this analysis, we explore the underlying physics of our solar cell by investigating essential parameters and equations, each represented by specific symbols to denote various physical quantities. The electrostatic potential is denoted by ψ, while ε0 represents both the relative permittivity of the semiconductor and the permittivity of free space. The concentration of free carriers is represented by p for holes and n for electrons. The densities of ionized acceptors and donors are denoted by NA− and ND+, respectively. Additionally, ρdef indicates the density of defect charges. The rate of photo-generation within the cell is symbolized by G, and R represents the net recombination rate.

4. Results and discussion

Figure 2(a) illustrates the I-V characteristics that were generated the KGeCI3 with MoS2 as ETL show the highest efficiency with 17.58%, as evidenced by the reduced values of defects in the absorber layer and interface. This device's current density is high, and its VOC is 0.77 v, as shown in the figure. Figure 2 (b) illustrates the quantum efficiency of the structure that was attained. The quantum efficiency (QE) ranging from 450 to900 nm is 90 percent. Thereafter, the QE decreases to 89 percent due to the narrow band gap of the perovskite, which did not absorb in the visible spectrum. However, the QE reaches zero at a wavelength greater than 900 nm, as this wavelength falls below the absorber layer bandgap.

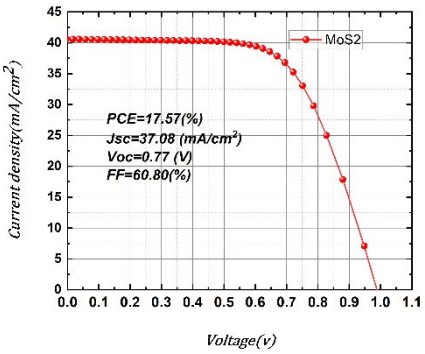

Figure 2. IV curve

5. Effect of ETL doping

Figure 5 illustrates the impact of the doping concentration in the ETL layer. The figure illustrates that at minimal donor densities, the power conversion efficiency (PCE) initiates at around 25%. As donor density escalates, the PCE swiftly rises to about 28% within the range of 2×10^{19} to 4×10^{19} cm^{-3}. Upon reaching this juncture, the PCE incrementally escalates at a diminished pace, nearing a peak value of around 29.5% as the donor

density attains 1×10^{20} cm^{-3}, akin to the increase in Voc and FF with increased concentration. This phenomenon mostly results from the improved collecting technique. The donor density significantly affects the power conversion efficiency (PCE), demonstrating an optimal range where efficiency increases considerably, followed by a region where further increases in donor density provide minimal efficiency improvements. In contrast Jsc significantly diminishes at reduced donor densities but stabilizes above a certain threshold, exhibiting a little increase as donor density further escalates. This indicates that an excess of donor atoms may initially hinder current generation, but the impact diminishes with elevated densities.

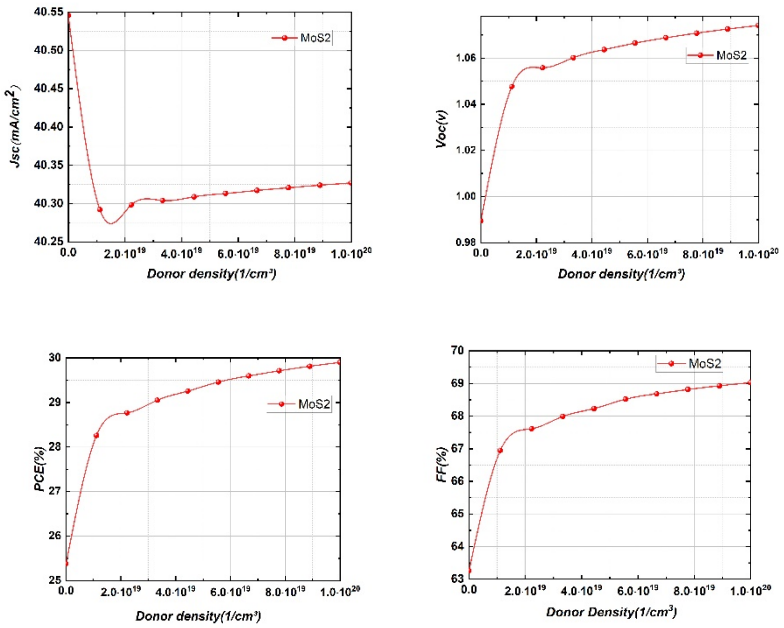

Figure 4. Effect of ETL doping Density

5. Conclusion

This study offers an extensive examination of the efficiency factors in KGeCl3 perovskite solar cells utilizing MoS2 as the electron transport layer, underscoring Doping ETL impact on performance. Through systematic optimization of material characteristics and resolution of interface challenges, we attained significant improvements in solar cell performance. The improved design resulted in a short-circuit current density (JSC) of 37.08 mA/cm², an open-circuit voltage (Voc) of 0.77 V, and a fill factor (FF) of 74.38%, achieving a potential efficiency of 15.49%. The results indicate significant possibilities for enhancements in 2D perovskite solar cells with focue doptimization. Our findings identify

critical elements influencing performance and establish a foundation for future.

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