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Perovskite solar cell simulation based on perovskite $CH_3NH_3PbI_3$ through SCAPS-1D simulation software

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Abstract
Photovoltaic energy production in solar cells can reduce our dependence on fossil fuels and toxic greenhouse gas emissions. Perovskite solar cells are, although lower in energy conversion efficiency, compare to any other types of solar cells. But, they have certain advantages such us low weight, flexibility and high absorption, and the process related to their preparation are has less expenses and lower complexity than silicon solar cells. These devices are composed of three main components: photo anode, active materials and cathode. In this article we have used $CH_3NH_3PbI_3$ as the active ingredient and optimized it with SCAPS simulation software.

Keywords: perovskite, solar cells, simulation, efficiency, SCAPS-1D

Introductions
In today's world, the economic growth of countries depends on the supply of energy resources. In most countries these resources include coal, oil, natural gas, and nuclear energy. Thus, the use of these resources faces several challenges, including the depletion of fossil fuel resources. Global energy consumption is projected to grow by more than 50% annually between 2003 and 2030. A similar increase in CO_2 emissions from combustible fossil fuel is projected. Therefore, in order to reduce the global reliance on finite natural resources and destructive fuels of the human environment we have shifted to renewable energy. During these years, many scientific efforts have been made to reduce costs and pollution for energy supply from renewable sources such as: solar energy, water, wind, geothermal etc. has taken place. In the meantime, due to clean and easy access to sunlight, solar energy is the best option for energy supply. What is ideal and coast effective is the acquisition of high-efficiency solar cell fabrication technology that converts solar energy into electrical energy and low manufacturing costs [1]. In this article we have studied and simulated $CH_3NH_3PbI_3$-based pervoskite solar cells.

Materials and Methods
The chemical formula of pervoskite is ABX_3, in which X is usually halogen (Br, Cl, I). Since X is a monovalent anion, A and B are cations of different sizes. A is usually CH3NH3 and B often lead (Pb) or tin (Sn) [2]. In recent years in the field of electronic devices Organometallic Perovskite Halide (PSC) solar cells have attracted the attention of the research community due to the simple processing technique and low manufacturing costs compare to traditional silicon-based solar and high PCE [3]. Organic-inorganic halide perovskite solar cells, the most common of which is a lead-iodide, organic-inorganic hybrid ($3CH_3NH_3PbI_3$) have excellent optical properties including high-absorption coefficient and energy gap.
Properly these compounds are suitable for light-absorbing applications. Methyl ammonium lead iodide is an am bipolar semiconductor compound that can transfer both electrons and cavities to the respective collecting electrodes. The low cost and simplicity of the process make this compound very suitable for use in high efficiency and cheap third generation solar cells. These pervoskite are made of two parts, organic and inorganic, methyl ammonium iodide as an organic part, and Lead and Tin are used as minerals. Perovskite solar cells has increased from 3.8 in 2003 to 25 in 2019. This increment is because of their good efficiency but Lead and Tin are problematic due to their toxicity in the same construction and the same time period [4]. In this simulation, SCAPS software or Solar Cell Capacitance Simulator which is a simulation software is used. It is a one-dimensional solar cell and was developed in the Department of Electronic System and Information (ELIS) by the University of Ghent,

Belgium. This software SCAPS is used for the simulation of this Low si/$CH_3NH_3PbI_3/TiO_2$ numeric model. We used Table 1 for Simulation.

Results and Discussions

PSC simulations were performed using SCAPS-1D under 1.5 AM sunlight and standard conditions. The results are shown in table 2. The $CH_3NH_3PbI_3$ perovskite despite being toxic, has an acceptable efficiency and it can be a good choice for perovskite solar cells due to its easy manufacturing method. The current voltage diagrams and quantum efficiencies are shown in figure 1 and 2 respectively.

Table 1: Simulation of Low si/$CH_3NH_3PbI_3/TiO2$ numeric model

Parameter	Low Si	$CH_3NH_3PbI_3$	Tio_2
Thickness	20	350	80
Eg (eV)	1.12	1.5	3.2
X (eV)	4.050	3.9	4.2
ε/ε0	11.9	10	10
Nc (cm^{-3})	1 x 10^{19}	1 x 10^{19}	2.5 x 10^{19}
Nv (cm^{-3})	1 x 10^{19}	1 x 10^{19}	2.5 x 10^{19}
μe (cm^2/V_s)	1.5 x 10^3	0.5	20
μh (cm^2/V_s)	4.5 x 10^2	0.5	10
ND (cm^{-3})	0	1 x 10^{18}	2.9 x 10^{20}
NA (cm^{-3})	1.5 x 10^{22}	1 x 10^{18}	0
Ve (cms^{-1})	1 x 10^7	1 x 10^7	1 x 10^7
Vh (cms^{-1})	1 x 10^7	1 x 10^7	1 x 10^7

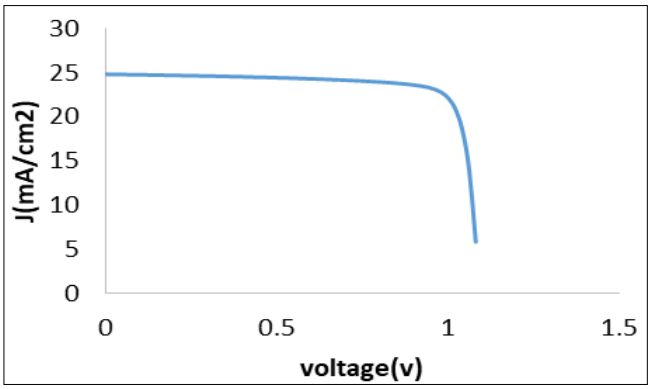

Fig 1: The current voltage of diagrams

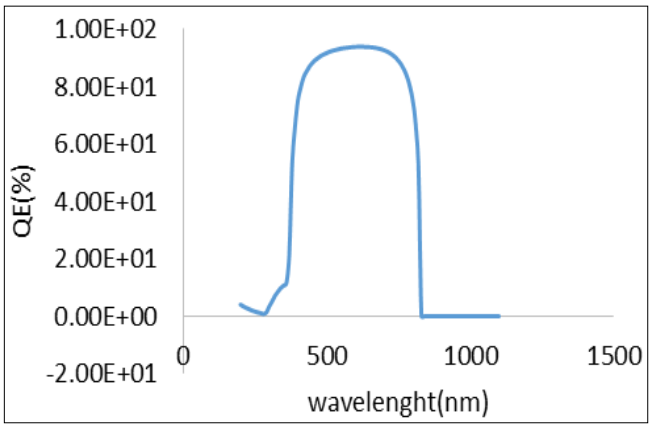

Fig 2: Quantum efficiencies

Table 1: Result of simulations performed using SCAPS-1D

Parameter's	Voc, v	Jsc, mA/cm^2	FF, %	PCE, %
With Graphene	1,089	24, 80	82, 45	22, 28

Conclusions

Through optimizing the thickness of the layers, creating defects in the electron transfer layers and electron collecting layers, we were able to achieve an efficiency of 22.28% under standard conditions. The Pervoskite Solar Cells have attracted the attention of many researchers due to its lower weight and easy composition. Therefore, this study could pave the way for the optimal design of high performance.

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