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Analysis of Lead-free Perovskite solar cells

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Abstract - *The performance of solar systems based on organic-inorganic halide perovskite materials has rapidly improved, and they are rapidly approaching commercialization. Lead-free perovskites have recently gotten a lot of press as a potential replacement for harmful lead-based compounds. We present the optimized version here. Numerical simulations of a methylammonium tin iodide (MASnI3)-based perovskite solar cell simulation. Different important characteristics, such as hole transport layers (HTLs) and doping, have an impact. The impact of density, thickness, and fault density on device performance is thoroughly investigated by using numerical simulation. The hole in the optimal device architecture is copper (I) oxide (Cu2O) and TiO2 as the electron transport layer, the maximum power conversion efficiency of 27.43 percent is achieved. The current density in the short circuit is 25.97 mA/cm2, the open-circuit voltage is 1.203 V, and the fill factor is 87.79 percent. This suggests that by tweaking device settings, high-performance lead-free perovskite solar cells could be achieved experimentally in the future.*

Key Words: Efficiency, Solar Cell, Perovskites

1. INTRODUCTION

Perovskite solar cells (PSCs) have proven to be one of the most promising. Power conversion efficiency (PCE) Over 25% on a single junction architecture, this can be difficult if it is a conventional silicon solar cell and is moving toward commercialization. Only over 10 years after its founding. But the road to the industrialization of PSC a handful of serious factors like device stability in the air below Lighting and toxicity of the materials used. Almost so far Successful compositions for perovskite solar cells Methylammonium (CH3NH3 +) (MA), formamidinium (NH2CHNH2 +) (FA), and A cation site cesium (Cs +), B cation site lead (Pb), and ABX3 Perovskite structure X anion site iodine (I), bromine (Br) [Five]. However, the presence of toxic heavy metals such as lead is associated with it. The entire life cycle of perovskite solar cells is a major concern from an environmental point of view. Therefore, the next high Efficiency, yet more research communities and industrialists doubt its future paving the way for lead-free perovskite material. That's why researchers are trying to study lead-free perovskite. Material for solar cells. Many lead-free perovskite absorbers. The material has a wide bandgap and is suitable for replacement. Toxic lead, including perovskite.

Further improvement in tin-based perovskite solar cells can be achieved by optimizing numerous parameters as well as device configurations, which can serve as a guide for future research. More enhancement through experimentation. This simulation work has resulted in a perovskite-based on methylammonium tin iodide (MASnI3) has been developed. Factors like as the thickness and doping levels of different layers, such as the electron layers of transport, perovskite absorber layer, and hole transport layer have been altered, and their consequences have been considered further performance enhancement defect densities have also been increased. Maximum achievable efficiency is 27.43%, which is the greatest reported to date. Any simulation method will yield a value in this scenario.

2. Methodology

Comprehensive research was conducted during this simulation work. For MASnI3 as a light absorption material. A negative feature of this material, which has been attracting attention in recent years, is this work. Unlike lead-based perovskite materials, it has non-toxic properties. MASnI3 can be a viable and high-contrast alternative to MAPbX3. The created configuration is one of the most important aspects of the simulation. It will be executed. This task will perform a device simulation Cleavage configuration of FTO / TiO2 / MASnI3 / HTL / Au. shown In the figure. 1. Light passes through the FTO edge and MASnI3 is Adopted as the main light absorption layer sandwiched Fluoride-doped tin oxide (FTO) is used between ETL and HTL Gold (Au) as front and rear metal contacts.

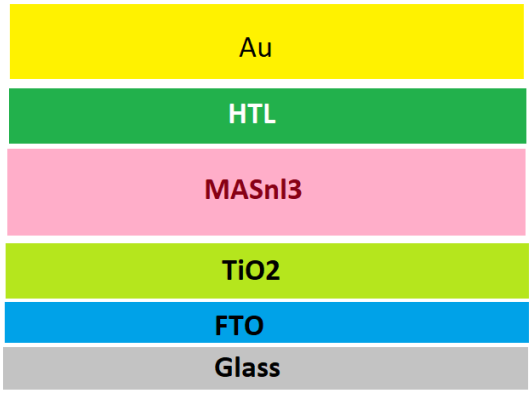

Fig.1- Schematic structure of the simulated PSCs,

This study focuses on simulating the configurations and various properties. The thickness of the various layers is input during the simulation. Doping concentration, electron and hole mobility, thermal velocity, Bandgap, electron affinity, permittivity, conduction. Effective state density of conduction band (CB) and Valence band (VB). Study the most suitable optical and electrical properties to achieve high power conversion efficiency. Various types of solar cells can be configured varies up to 7 layers. Equations related to the calculation of output and follow Poisson's equation for a semiconductor labeled as follows:

$$\nabla^2\psi = q/\varepsilon\ (n - p + M_A - M_D)$$

Where M_A is the acceptor concentration and M_D is the donor concentration. ψ is the electrostatic potential. Semiconductor continuity equation.

$$\nabla.J_a - q\ (\partial n/\partial t) = +qR$$

$$\nabla.J_b + q(\partial p/\partial t) = - qR$$

Here, J_a represents the current density of electrons, and J_b represents the current density of electrons. The hole current density and R are the carrier recombination rates. There are two common effects that govern the flow of current in a semiconductor. First, there are the minority charge drift carriers due to the influence of the electric field and secondly, diffusion power is generated by the concentration gradient. Drift - diffusion current relationship is given by the continuity equation.

$$J_a = qn\mu_n E + qD_n \nabla n$$

$$J_b = qp\mu_p E - qD_p \nabla p$$

Photovoltaic devices have three main parts: Light absorber Charge carriers, or layers that convert incident photons into electrons and holes, carrier collectors for capturing carriers, and metal contacts to them charge carriers transferred to an external circuit. The absorber used here is $MASnI_3$. The simulation was derived from various other research papers. Those references are quoted. Table 1 shows a list of the following values: Considered when first forming the basic configuration Simulation process to obtain optimized results through variations.

Material property	TiO_2	$MASnI_3$	Cu_2O	Spiro-OMeTAD	NiO	CuI	PTAA
Thickness (nm)	Varied	varied	varied	200	200	200	200
Band gap (eV)	3.2	1.3	2.17	2.88	3.8	3.4	2.96
Electron affinity (eV)	4	4.17	3.2	2.05	1.4	2.1	2.3
Dielectric permittivity	9	6.5	7.5	3	10.7	10	9
CB effective density of states (cm^{-3})	2×10^{10}	1×10^{18}	2×10^{18}	2.2×10^{18}	2×10^{19}	2.5×10^{18}	1×10^{21}
VB effective density of states (cm^{-3})	1.8×10^{19}	1×10^{19}	1.8×10^{18}	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	1×10^{21}
electron thermal velocity (cm/s)	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}
hole thermal velocity (cm/s)	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}
Electron mobility ($cm^2/V.s$)	20	1.6	20	2×10^{-4}	12	2×10^{4}	1
Hole mobility ($cm^2/V.s$)	10	1.6	80	2×10^{-4}	28	2×10^{4}	40
Shallow donor density N_D (cm^{-3})	Varied	–	–	–	–	–	–
Shallow Acceptor density N_A (cm^{-3})	–	varied	varied	2×10^{19}	2×10^{19}	2×10^{19}	2×10^{19}
Defect density N_t (cm^{-3})	1×10^{15}	2×10^{15}	1×10^{14}	1×10^{15}	1×10^{14}	1×10^{15}	1×10^{14}

Table 1 - Values representing the material properties used in the simulation

3. Result and Discussion

The simulation was performed based on tabular parameters Collected from various theoretical and experimental studies. every day The components of perovskite solar cells are Device performance. Various hole transport layers have been used FTO / TiO_2 / $MASnI_3$ / HTL /Au device configuration keeps everything the same parameters. Variations help determine the performance of device models with different HTLs. The decisive factor in selecting the best material for HTL. The J-V characteristics of PSC simulated using copper (I).Oxide (Cu_2O), copper iodide (CuI), nickel oxide (NiO), poly [bis (4) Phenyl) (2,4,6 trimethylphenyl) amine (PTAA) and 2,2', 7,7'tetrakis (N, Ndi4 methoxyphenylamino) 9,9'-spiromeOTAD. The performance of devices using Cu2O Compared to others. Performance parameters obtained after simulation Table 2 shows the use of different HTLs.

Performance parameters	NiO	CuI	Spiro-OMeTAD	Cu_2O	PTAA
Open circuit voltage (V)	0.924	0.934	0.924	0.934	0.924
Short circuit current density (mA/cm^2)	27.40	28.50	26.90	28.62	27.09
Fill factor (%)	77.99	80.41	67.19	80.35	77.83
Efficiency (%)	19.75	21.42	16.71	21.48	19.48

Table 2 - performance parameters with various HTLs.

The efficiency of CuI is very close to Cu_2O the corresponding QE spectrum of a PSC with a different HTL matches the characteristics of the J-V. PSC using Cu_2O as HTL shows a higher short circuit current in the 400-600 nm range compared to others. expensive performance of perovskite solar cells using CuI or Cu_2O as the HTL layer of all other hotels, it is mainly due to its high mobility/conductivity. This copper-based inorganic p-type semiconductor, and also The maximum values of the valence bands of these materials are well aligned Active perovskite absorption layer. Based on

overall performance Cu_2O was used as the HTL to further optimize performance. The thickness of the Cu_2O layer was defined by FTO / TiO_2 / $MASnI_3$ / Cu_2O / Au device configuration. Figure 3a shows the plot of Performance parameters as a function of HTL thickness. Have been observed All parameters remain nearly constant or increase slightly the layer thickness increases from 10 nm to 100 nm. Optimizing the electron transport layer is also very important for achieving higher photovoltaic performance in perovskite Solar cell.

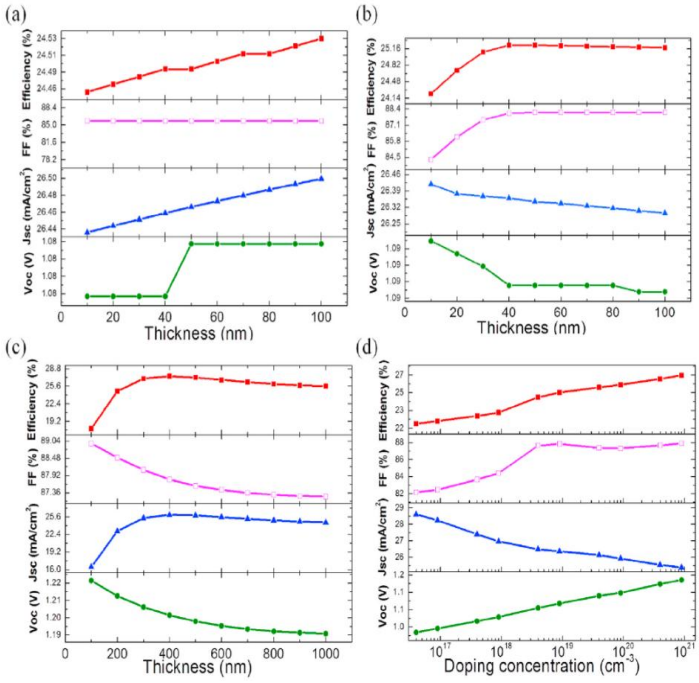

Fig. 3. Variation of performance parameters (VOC, JSC, FF, and efficiency) of PSC with different, (a) HTL thickness, (b) ETL thickness, (c) perovskite layer thickness, and (d) doping concentration in the perovskite layer.

Optimizing ETL gives you control over pricing Perovskite solar cell recombination rate. Figure 3b shows the figure. Performance parameters as a function of changing ETL thickness in the range of 10-100 nm. A very slight decrease was observed when the layer thickness increases with the open-circuit voltage, after a period of time, a slight decrease follows, which may be due to an increase. Recoupling with series resistance in the device. The VOC obtained is 10 nm and the value is about 1.09 V. Short circuit Current density (JSC) initially decreases slightly as it increases Thickness, and JSC decreases according to a nearly linear curve, Get the minimum value with a thickness of 100nm ETL. The curve factor (FF) and efficiency curve show similar properties. Both gain thickness varies from 10 nm to 40 nm. As the thickness increases, the FF and PCE become nearly constant.

Ignore fluctuations. Therefore, for optimal configuration, ETL thickness ranges from 40 nm to 60 nm and should be about the same for carrier diffusion length. The thickness of the absorber layer plays a very important role in determining the quality of the absorber layer and the performance of the thin-film Solar cell. Figure 3c shows various plots showing the impact. Performance parameters due to fluctuations in the thickness of the absorber layer 100 nm to 1000 nm by keeping other optimized parameters the same. The VOC and FF of the device are the thickness of the perovskite layer. Exciton generated by photon absorption Cannot exceed the depleted barrier potential Layers that can lead to higher recombination rates of charge carriers and higher reverse saturation currents lead to lower VOCs. Both JSC and PCE increase as the thickness of the perovskite layer increases. Up to 400 nm, then both decrease with increasing layers thickness. As the thickness of the perovskite layer increases, the active one becomes the first increases absorber area and promotes more exciton generation as a result, JSC, and PCE, increase. But it keeps increasing thickness leads to higher resistance (also higher defects, higher rejoin rate), which leads to a decrease in each value. Indicates the efficiency is more affected by the value of JSC. VOC values have a greater effect on JSC than absorber thickness VOC. Therefore, all factors need to be considered to choose the best absorber thickness. Various experimental studies have already been done showing that the performance of solar cells is highly dependent on perovskite. Layer morphology directly affects the photogenerated support Lifespan and diffusion length. Therefore, it is very much essential to control the doping density in the perovskite layer to optimize the performance. The influence of doping density levels in the perovskite materials in solar cell performances was also studied which shows the influence of different parameters on changing the doping levels of the perovskite material which are shown in Fig. 3d. As the doping concentration (acceptor impurity) is increased the VOC, FF, and PCE also gradually keep increasing. As the doping density increases, JSC decreases due to increase in recombination of photogenerated charge carriers in the perovskite materials that leads to decrease in minority carrier concentration, carrier mobility, and minority carrier diffusion length. The VOC of solar cell depends on the following equation:

$$VOC = (nkT/q)\ln(J_{SC}/J_O+1)$$

Where, k is Boltzmann`s constant n is the ideality factor, J_o is the reverse saturation current density, T is temperature, and q electronic charge. It is very clear that the VOC value is highly dependent on J_{SC} and the reverse saturation current density. As we can see that the short-circuit current density decreases with an increase in doping. So, if the VOC increases even at decreasing JSC, then it`s definite that the reverse saturation current must be decreasing at a higher rate with the increase in doping than JSC, which adds on to the increase in VOC. This may be due to the fact that an increase in the doping concentration results in higher conductivity which helps in obtaining a higher built-in potential

ultimately leads to higher VOC. So, an optimum doping level can be determined by looking at all these doping impacts. Finally, based on the optimized parameters of each PSC component, the overall performance of is simulated.

Fig. 4a shows the energy band diagram of PSC with Cu_2O as hole transport layer. The JV characteristics of lead free MASnI3 based solar cell in the optimized device configuration under dark and illumination conditions is shown in Fig. 4b. The values of optimized parameters are JSC = 25.97 mA/cm2, VOC = 1.203 V, FF = 87.79%, and PCE =27.43%. Fig. 4b (inset) shows the quantum efficiency curve in different wavelengths of the same device with a maximum QE value of 89.2%. The generation and recombination depth profile of the charge carrier is shown in Fig. 4c. The generation of charge carriers is high at the interface between TiO2 and perovskite, low carrier recombination on the other hand, in the case of the interface between Cu_2O and perovskite, is generated. There is less carrier recombination. Therefore, from this simulation work, all the components and their respective parameters are clear. It plays an important role in improving the performance of the device.

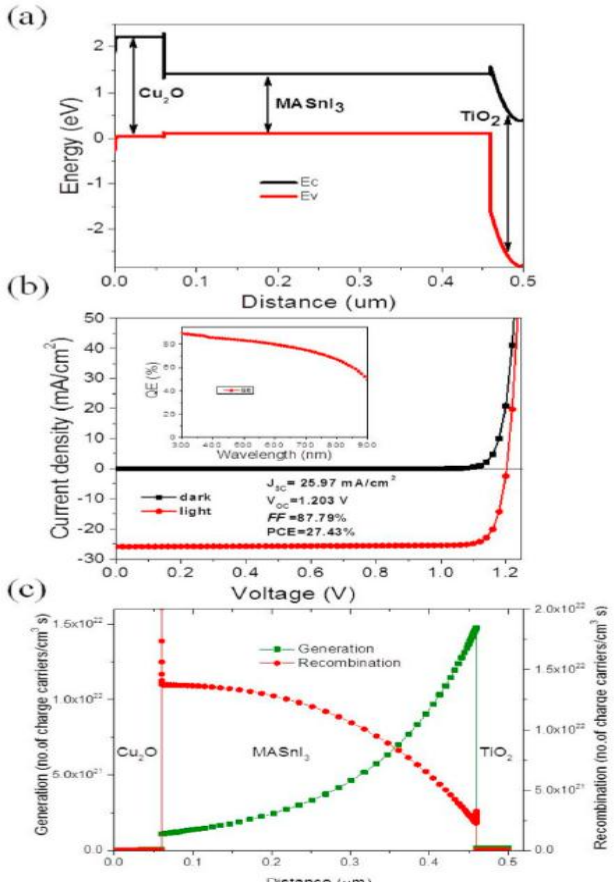

Fig. 4. (a) The energy band structure diagram of PSCs, (b) optimum device J-V curve in both light and dark conditions, inset QE curve, (c) generation and recombination rate with depth profile in the optimum device configuration.

4. Conclusion

In summary, the optimization of lead-unfastened $MASnI_3$ primarily based on totally perovskite sun mobileular overall performance became very well-investigated the primarily based totally numerical simulation. The effect of diverse HTLs at the tool overall performance became studied to get the high-quality viable efficiency. It became found that tool with TiO_2 as ETL and Cu_2O as HTL confirmed better overall performance in comparison to the opposite devices. We have optimized one-of-a-kind residences like doping density, the thickness of lively materials in addition to hollow and electron shipping layer HTL and ETL for the in-addition development of the tool's overall performance. Moreover, it's been found that the various HTL thickness has a minimum effect at the tool operation and its overall performance, while the thicknesses of ETL and absorber layers appreciably effect the tool parameters. Secondly, the doping of the lively layer performs a primary function withinside the tool`s overall performance. So far, the best Perovskite cell efficiency of 27.43% became received through this simulator the usage of $MASnI_3$ materials. This modelled tool shape may honestly manual the studies groups for in addition exploration in lead-unfastened perovskite primarily based totally sun cells.

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