

A study of Simulation of Perovskite based Solar Cell

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Abstract

A CH₃NH₃PbI₃-xCl_x perovskite based device has been simulated to analyze its performance as solar cell and photodetector. The device shows high power conversion efficiency and open circuit voltage as a solar cell. It is shown that the thickness of perovskite absorber and the choice of electrode material have significant impact on the performance of the perovskite solar cell. The maximum power conversion efficiency of 22.7% and open circuit voltage of 1.13V is obtained after optimization of the device parameters. The same device also shows impressive response as a photodetector. It achieves maximum responsivity of 0.45 A/W at a wavelength of 600 nm and a detectivity of 6.01×10¹¹ Jones for perovskite absorber thickness of 500 nm. Effect of bulk and interface defects of perovskite absorber film on the performance of photodetector has also been studied. The results show that the perovskite device is a suitable candidate for both the solar cell and photodetector applications.

Keywords: Perovskite, Solar Cell, Photodetector.

I. INTRODUCTION

Organometal halide perovskite materials like CH₃NH₃PbI₃ and CH₃NH₃PbBr₃ have been widely explored for photovoltaic applications in the last few years. Perovskite refer to the class of materials which can be represented by a general formula ABX₃, where A is a big size cation, B is a small size divalent metallic cation and X is a halide ion. Presently extensive research is ongoing in the development of perovskite based photovoltaic devices. Kojima et al reported the first application of perovskite as a photosensitizer in 2009[1]. This work motivated many other researchers to explore perovskite materials for various photovoltaic applications. Since then huge progress has been made in the field of perovskite based photovoltaic applications. Various types of structures have been proposed for the perovskite solar cell [2-5]. Due to these efforts perovskite solar cells currently outperform many other solar cells based on organic and inorganic materials in terms of power conversion efficiency [6-7]. Perovskite materials possess some special properties like high optical absorption coefficient, large carrier mobility and large carrier diffusion lengths that make them very attractive for photovoltaic applications [8-11]. Moreover the perovskite thin films can be synthesized using low temperature solution processing techniques and it is also possible to deposit the thin films of perovskite on flexible substrates. This makes the perovskite based devices economical and also allows them to be used in flexible electronic devices. Device simulation is an effective medium to gain more insight into the principles of operation of electronic devices which help to further improve their performance. In this paper we have simulated CH₃NH₃PbI₃-xCl_x based perovskite device to analyze its performance as a solar cell and photodetector using SCAPS (Solar Cell Capacitance Simulator) software. SCAPS is a 1-dimensional simulation software which calculates energy bands, current-voltage characteristics and spectral response (Quantum Efficiency) by solving continuity equations for electron and hole and Poisson's equation. compared with other organic and inorganic photodetectors reported in the literature.

PEROVSKITE DEVICE AS SOLAR CELL

In this section we explain the simulation of the proposed perovskite device as a solar cell. Here we have also explained the principle of operation of the perovskite device solar cell and the analysis of simulation results.

Device Structure and Simulation Parameters

Fig. 1(a) and (b) shows the structure of the device used in the simulation and the energy band diagram corresponding to this device. The device consists of a thin film of perovskite CH₃NH₃PbI₃-xCl_x sandwiched

between FTO (Fluorine doped Tin Oxide) coated glass and gold electrode. Light enters the device from the FTO side and large number of photons are absorbed in the perovskite layer (due to high optical absorption coefficient of the perovskite material). The photons energy is utilized to generate free electrons and holes in the perovskite absorber layer. These electrons and holes are separated and then collected on the two electrodes to give rise to photocurrent. Due to large diffusion length of the perovskite material, loss of photogenerated carriers due to recombination is very small in the perovskite absorber layer which helps to increase the power conversion efficiency of the perovskite device.

The material parameters of each layer are chosen from the literature [2,16] and are listed in Table 1. ND is donor concentration, ϵ_r is relative permittivity, χ is electron affinity, E_g is bandgap, μ_n and μ_p denote electron and hole mobility, N_t is defect density and N_C and N_V are effective density of states of conduction band and valence band, respectively. Other simulation parameters are: thermal velocity of electron and

hole is 107 cm/s, capture cross section of electron and hole is $2 \times 10^{-14} \text{ cm}^2$. Defect energy level is centre of E_g and defect type is neutral. Gaussian energetic distribution with the characteristic energy equal to 0.1 eV is used in the simulations. The light source illuminates the device from FTO side. The thickness of FTO is 500 nm. Optical absorption coefficient α , is calculated by $\alpha = A [h\nu - E_g]^{1/2}$ where constant A is taken to be equal to 105. SCAPS software has been used for simulation work. SCAPS has been extensively used for the simulation of CIGS and CdTe solar cells and the results are in good agreement with experimental results [12-14]. In the last few years many works of SCAPS simulation of perovskite solar cells have been reported [15-17]. Since the excitons in the perovskite material are of Wannier-type with binding energy of 50 meV, we can deal with their photo-excited carriers in the same way as in the case of inorganic materials like CIGS and CdTe [18-19].

Firstly the performance of the perovskite device as a solar cell has been explained in the previous of the paper and secondly the performance analysis of the same perovskite device as a photodetector has been presented in the section previous of the paper. The perovskite device presented in this paper has simpler structure than many other commonly reported perovskite solar cell device structures. Simulations have been done to optimize the performance of the device. The device exhibits fairly high Power Conversion Efficiency (PCE) making the device suitable for solar cell applications. Although many works of simulation of perovskite based devices have emerged in the last few years [20-22], but still there is lack of simulation study of perovskite based photodetectors. Here we have performed simulation study which shows that the perovskite based device proposed in this work can be an economical and efficient candidate for photodetector applications. Current-voltage characteristic obtained by simulation is used for the determination of responsivity of the device. The responsivity is high over a wide range of wavelength. Effect of perovskite thickness on the responsivity of device has been investigated to determine the optimum thickness of perovskite. The perovskite device exhibits high light current to dark current ratio along with high detectivity. Finally the photodetector parameters are



Fig.1(a). Perovskite device structure.

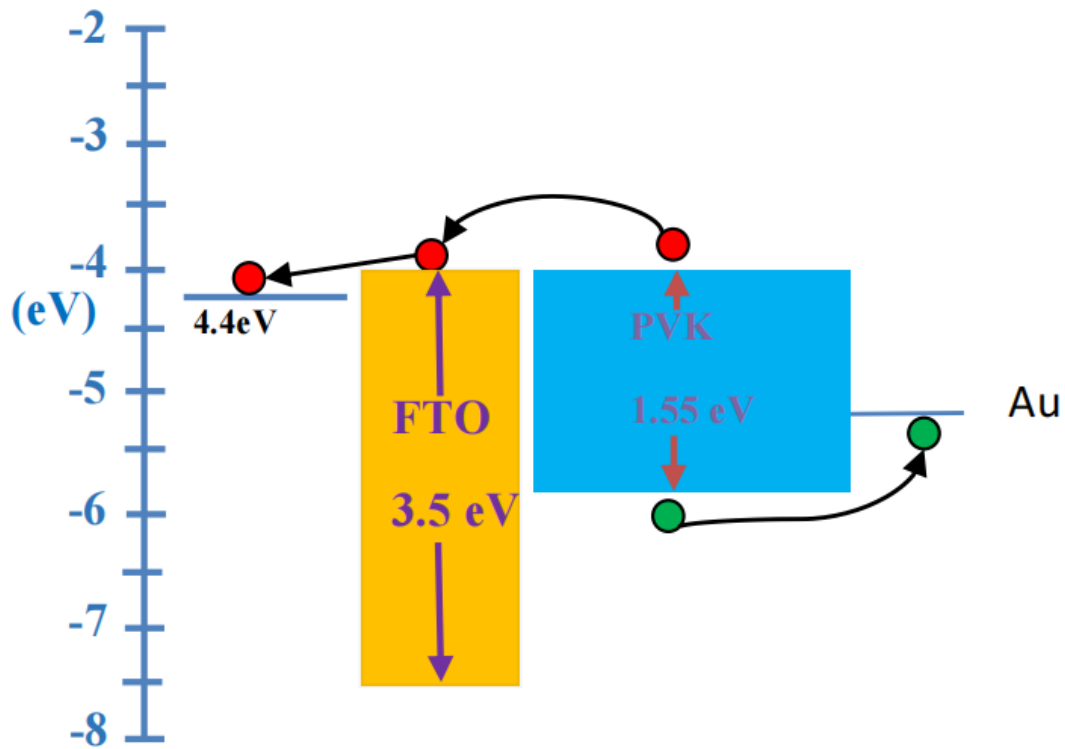


Fig.1(b). Energy band diagram of device (Perovskite is shown as PVK).

Table 1. Material Parameters used in simulation.

Parameters	FTO	Perovskite
ND(1/cm ³)	2×10 ¹⁹	10 ¹³
ε _r	9.0	6.5
χ (eV)	4.0	3.9
E _g (eV)	3.5	1.55
μ _n /μ _p (cm ² /V ^s)	20/10	2.0/2.0
N _t (1/cm ³)	10 ¹⁵	2.5×10 ¹³
N _c (1/cm ³)	2.2× 10 ¹⁸	2.2× 10 ¹⁸
N _v (1/cm ³)	1.8 ×10 ¹⁹	1.8 ×10 ¹⁹

II. Results and Discussion:

Fig. 2 shows the current density-voltage (J-V) curve of the device under dark and illuminated conditions. The standard AM 1.5 G spectrum has been used for illumination in the simulations. The J-V curve resembles a typical solar cell characteristic where power can be generated by operating the device in the fourth quadrant of J-V curve.

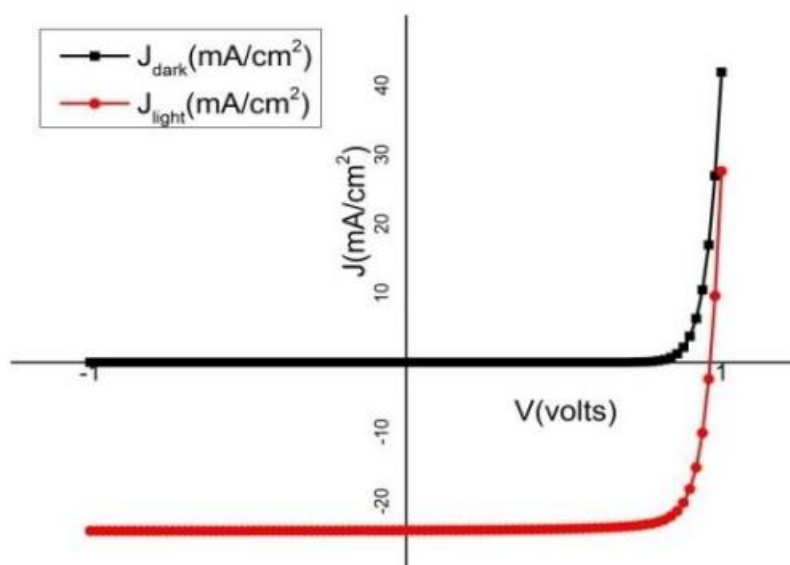


Fig. 2. J-V characteristic of Perovskite Solar Cell.

In order to optimize the performance of solar cell we have investigated the effect of different parameters on the device performance. Effect of perovskite thickness and effect of using different transparent electrode and metal electrode is evaluated with the help of simulations and the results are discussed below.

Effect of front and back electrode on Solar Cell Performance:

The Table 2 compares the performance parameters of perovskite solar cell by using FTO and ITO (Indium Tin Oxide) as the front transparent electrode. The perovskite absorber thickness is 500 nm and gold has been chosen as the back electrode in this analysis.

Table 2. Performance comparison of solar cell for different front electrodes.

Solar Cell Parameters	FTO	ITO
PCE(%)	18.01	13.64
Open Circuit Voltage(V)	0.933	0.889
Short Circuit Current(mA/cm ²)	24.25	24.37
Fill Factor (%)	79.60	62.97

It can be seen that the performance of the perovskite solar cell is much better in the case of FTO as front electrode. The Table 3 compares the performance of perovskite solar cell by using silver and gold as back electrode material while keeping FTO as front electrode. It is clear from the table that gold electrode is a better choice than silver electrode for this perovskite device as solar cell.

Table 3. Performance comparison of solar cell for different back electrode.

Solar Cell Parameters	Gold(Au) back contact	Silver(Ag) back contact
PCE (%)	18.68	3.06
Open Circuit Voltage(V)	0.96	0.24
Short Circuit Current(mA/cm ²)	24.25	23.70
Fill Factor (%)	79.85	53.26

The performance of the perovskite device using aluminium as back electrode was also studied. Fig. 3 shows the J-V characteristic of the perovskite device using aluminium as back electrode under illumination condition. It shows that the J-V curve is non rectifying and passes through the origin. Hence it is not suitable for solar cell application. This result can be explained by the fact that a metal/n-type semiconductor

junction forms a non rectifying ohmic junction when the work function of metal is less than the work function of semiconductor which is the case here as the workfunction of aluminium (4.1eV) is smaller than the workfunction of perovskite. These results are also consistent with the fact that most of the reported perovskite solar cells use FTO and gold as front and back electrode. From the above discussion it is clear that combination of FTO and gold electrode is best for this perovskite device therefore in the rest of the simulations we have used FTO and gold as front and back electrodes.

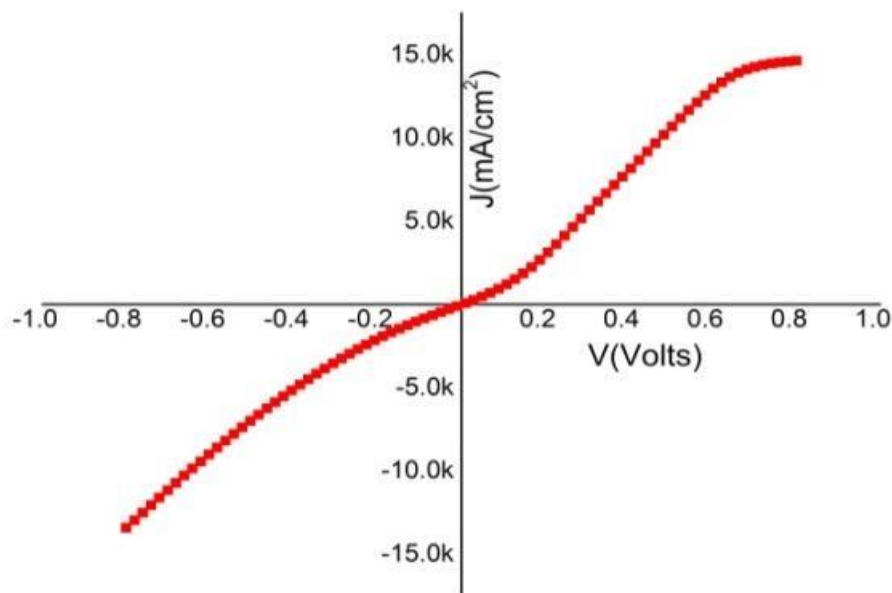


Fig. 3. J-V characteristic of Perovskite solar cell with Silver as back electrode.

Effect of Perovskite Thickness

The thickness of perovskite absorber film plays a very important role in the functioning of solar cell as the perovskite film absorbs the photons from the solar illumination and generates electric carriers. If the thickness is very small then the number of photons absorbed in the film is very low which results in the low power conversion efficiency and if the perovskite thickness becomes too large the recombination of photogenerated carriers increases which also results in the reduction of power conversion efficiency of the solar cell. Hence to find the optimum thickness of perovskite film the solar cell has been simulated for different thickness of the perovskite absorber. Fig. 4(b) shows the variation of power conversion efficiency of perovskite solar cell with the thickness of perovskite film and Fig. 4(a) shows the J-V

characteristics of solar cell corresponding to the maximum power conversion efficiency. It can be seen from the plots that at a perovskite absorber thickness of 2.3 μm maximum power conversion efficiency of 22.7% and open circuit voltage (Voc) of 1.13 V is obtained. Hence it can be said that the thickness of perovskite absorber should be set to 2.3 μm in order to achieve best performance from the solar cell.

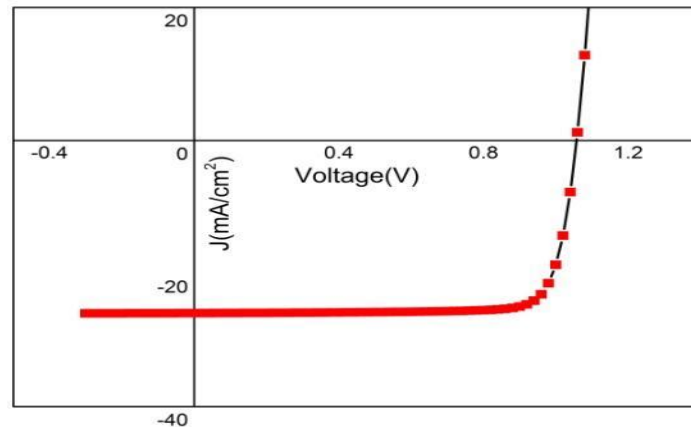


Fig. 4. (a) J-V curve for optimum perovskite absorber thickness of 2.3 μm .

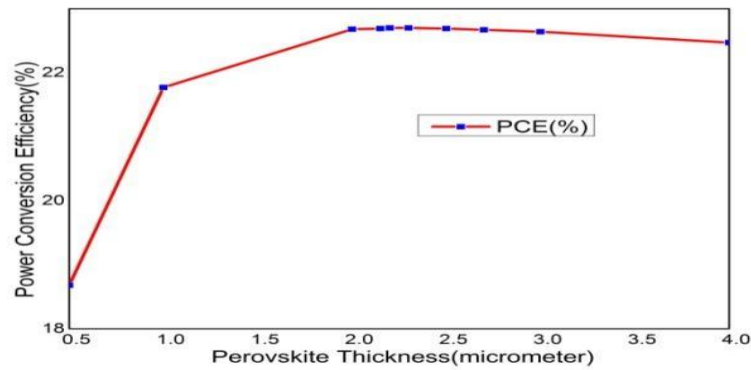
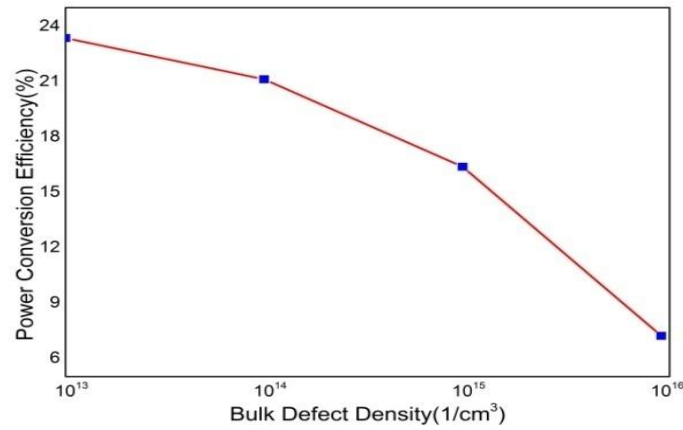


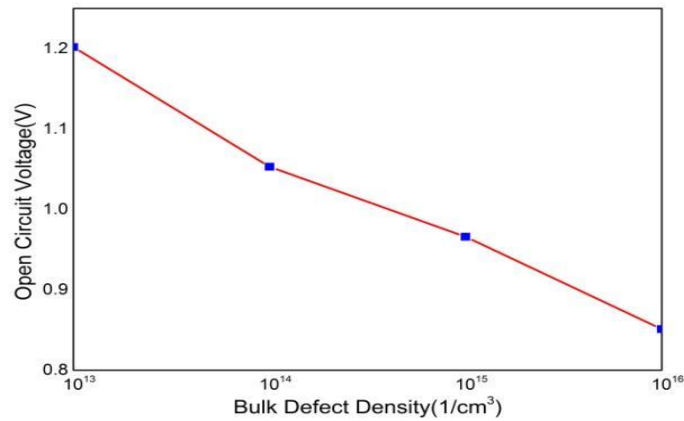
Fig. 4(b). Variation of Power Conversion Efficiency with perovskite absorber thickness.

Effect of Bulk defect density:

Fig. 5 shows the effect of bulk defect density of the perovskite film on the power conversion efficiency and open circuit voltage of the perovskite solar cell. It can be seen that both the PCE and V_{oc} gets reduced sharply as the bulk defect density increases. This is in concurrence with the report that increasing the crystallinity of the perovskite film reduces the trap density which leads to better performance of perovskite solar cells [26]. This happens because the defect sites act as recombination centres which reduces the number of photogenerated carriers. This shows that special care should be taken of the surface morphology of the perovskite film during fabrication of solar cell in order to improve the PCE.



(a)

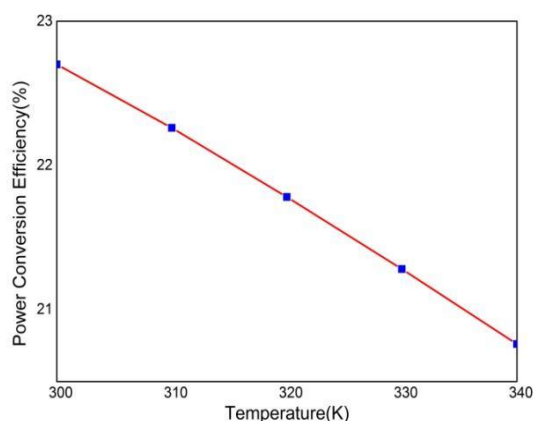


(b)

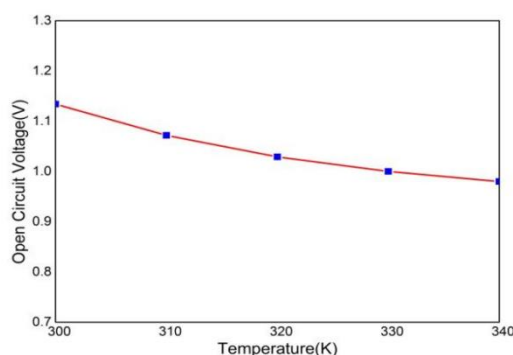
Fig. 5(a & b). Graphs showing variation of Power Conversion Efficiency and Open circuit voltage with the bulk defect density.

Effect of Temperature:

Solar cells are used in different geographical regions under different weather and climates over the year which changes the operation temperature of the Solar cell. To find the effect of temperature variation on the performance of the perovskite solar cell, simulations have been performed for different operating temperatures. Fig. 6 shows the effect of operating temperature variation on the solar cell performance. It is observed from the plots that the PCE and Voc decreases with the increase in temperature. Thus it can be said that the perovskite device gives better performance as solar cell at lower operating temperatures.



6(a)



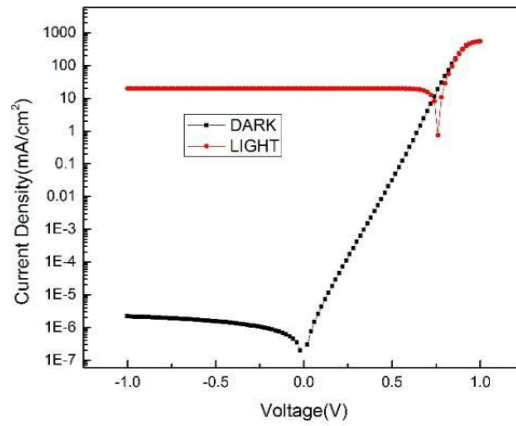
(b)

Fig. 6(a & b). Variation of Power Conversion Efficiency and Open circuit voltage with operating temperature. Thus it can be said from the above discussion that the proposed perovskite device shows high performance as a solar cell through proper optimization of various device parameters. In the next section we present the analysis of the same device as a photodetector.

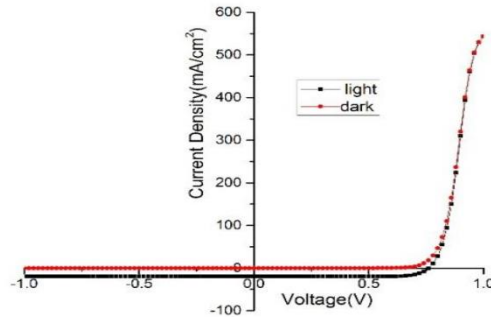
PEROVSKITE DEVICE AS PHOTODETECTOR

In this section we present the simulations which have been performed to evaluate and analyze the performance of the perovskite device as a photodetector. Fig. 1(a) shows the structure of the device simulated as a photodetector. The light input is from the FTO (front electrode) side and gold has been used as the back electrode. The perovskite absorber is sandwiched between the two electrodes. The light used for illumination in the simulations has a wavelength of 600 nm and intensity of 100 mW/cm². The other simulation parameters used in this case are same as used in the solar cell simulation of perovskite device as reported in section 2.1.

III. Results and Discussion:



7(a)



7(b)

Fig. 7. J-V curve under dark and illumination condition (a) Logarithmic plot (b) Linear plot.

Fig. 7(a) and (b) show the logarithmic and linear plots of current density-voltage (J-V) curve of the device under dark and illumination conditions. The reverse current density as obtained from the J-V curve under dark condition is estimated to be equal to 2 $\mu\text{A}/\text{cm}^2$. It is also observed from the plot that the dark J-V characteristic is highly rectifying (similar to a diode characteristic) which makes the perovskite device suitable for many other electronic applications.

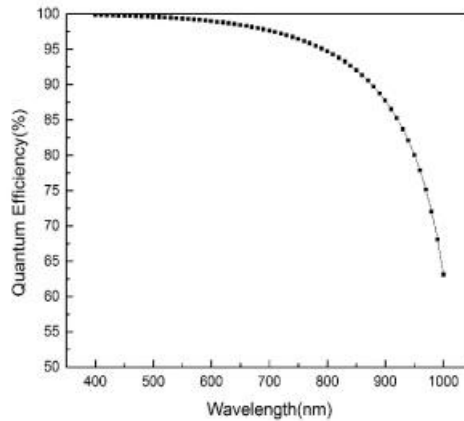


Fig. 8. Quantum Efficiency versus wavelength.

Under illumination condition the reverse current across the device gets increased significantly due to the presence of photo generated carriers. Photocurrent to dark current ratio as calculated from the J-V curve is found to be 9.16×10^6 at +/- 1V which is a fairly high value of photocurrent to dark current ratio for a thin film photodetector. Fig. 8 shows the quantum efficiency of the device obtained by simulation. Very high quantum efficiency is achieved which is due to the excellent optical properties of perovskite film. For higher wavelengths there is a fall in the quantum efficiency as the absorption coefficient of the material decreases at higher wavelengths. Responsivity of the device has been calculated from the following equation

$$R = \frac{q\eta\lambda}{hc} \quad (1)$$

where R is the responsivity of photodetector, η is the quantum efficiency, λ is incident light wavelength, $h=6.634 \times 10^{-34}$ Joule-second is the Planck's constant, $c = 3 \times 10^8$ m/s is the speed of light and $q=1.6 \times 10^{-19}$ C is the electronic charge. Fig. 9 shows the responsivity of the device as a function of wavelength. High value of responsivity is achieved over a wide range of wavelength which suggests the possible use of this device for practical photodetection applications. Thickness of the perovskite absorber film is an important parameter of the device which affects the overall performance of photodetector. Fig. 10 shows the variation of responsivity curve for different thickness of perovskite film. Responsivity of the device increases as the thickness of the perovskite film is increased from 200 nm to 900 nm. For shorter wavelengths, responsivity almost saturates beyond 500 nm thickness. For a perovskite thickness of 500 nm and the input light wavelength of 600 nm, the responsivity of the photodetector reaches a value of about 0.45 A/W and there is no major increment in the responsivity as the wavelength is further increased.

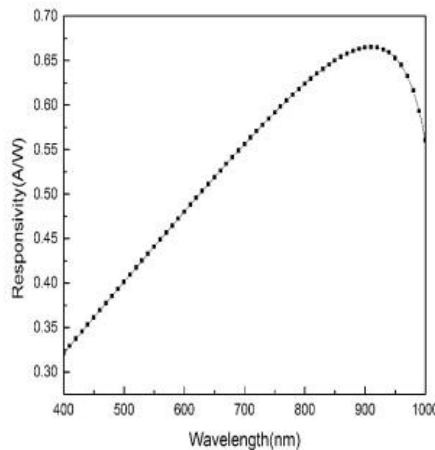


Fig. 9. Variation of Responsivity with wavelength.

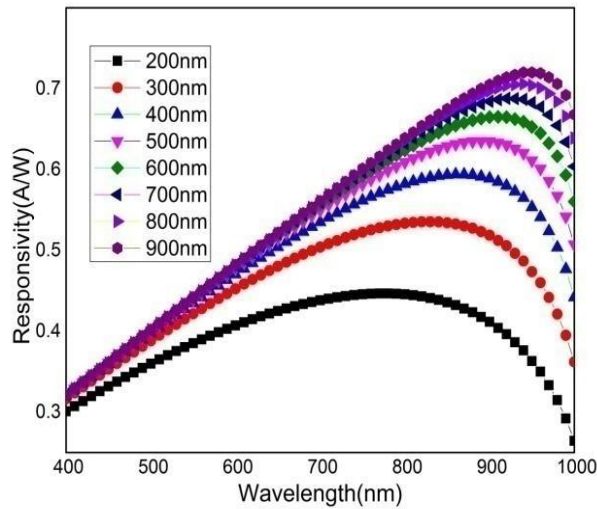


Fig.10. Responsivity variation with wavelength for different values of perovskite absorber thickness.

The detectivity as a function of voltage is estimated using the following equation:

$$D = \frac{R}{\sqrt{2qJ}} \quad (2)$$

□

where R is the responsivity of photodetector and J is the reverse saturation current density. The detectivity of the perovskite photodetector as calculated from the above equation turns out to be equal to 6.01×10^{11} Jones which makes the device suitable for practical photodetector applications.

Defects in the semiconductor can affect the performance of a semiconductor device to a large extent. Therefore in order to evaluate the effect of defect density on the responsivity of the device we have compared the responsivity of the device for various values of bulk and interface defect densities as shown in Fig. 11 and Fig. 12 respectively. It can be observed that the responsivity of the perovskite device photodetector gets reduced as the defect density increases. It is also observed that the effect of bulk defects is more prominent as compared to the interface defects. Thus it can be said that the quality of the perovskite film is a critical parameter for the performance of perovskite device photodetector.

Comparison with other photodetectors:

Table 4 shows the comparison of the perovskite photodetector parameters with some of the other types of photodetectors reported in literature. It can be observed from the table that the simulated device has better performance as compared to the other mentioned photodetectors. Moreover there are only few reports of perovskite based photodetectors till date in the literature. This is the first report of simulation study of perovskite photodetector as per our knowledge. It is expected that this work will help to motivate further research for the development of better perovskite based photodetectors. Finally we mention some sources of error in the simulation of perovskite device as solar cell and photodetector reported in this paper. Firstly we have not taken the actual value of transmission coefficient of FTO and assumed it to be 100 percent. Although in practice the transmission coefficient is lesser than one. Secondly we have not considered reflection from each layer and interface and additional series resistance from FTO and back contact assuming it to be very small. Therefore in order to get more precise results these factors should also be incorporated into the simulations.

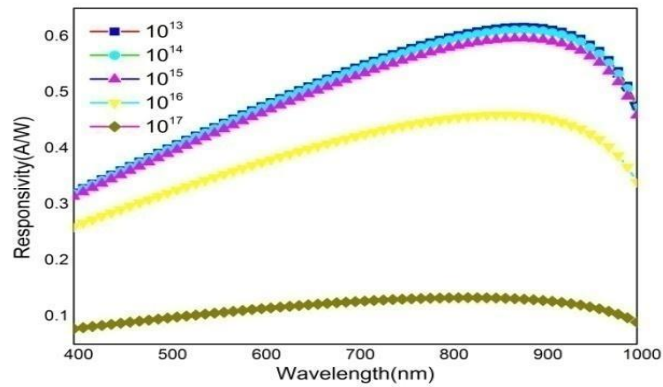


Fig.11. Responsivity variation with wavelength for different values of bulk defect density.

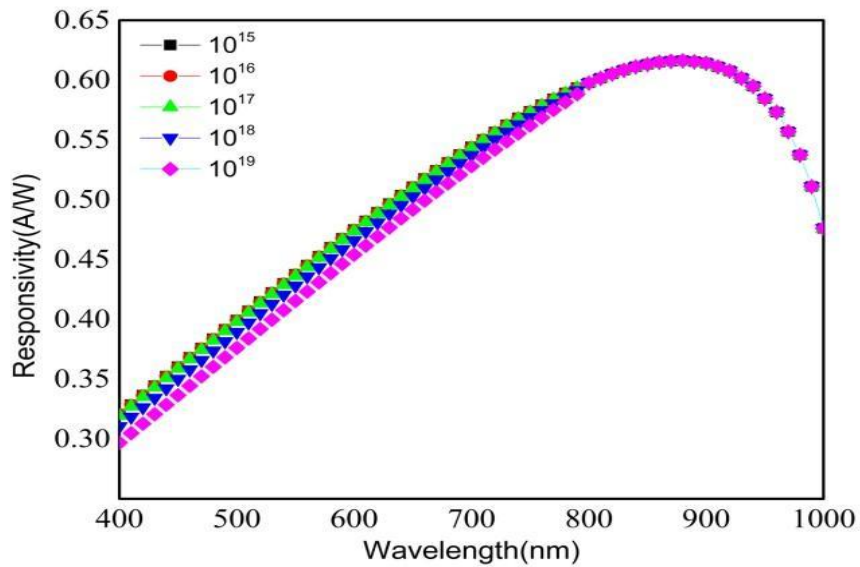


Fig.12. Responsivity variation with wavelength for different values of interface defect density.

Table 4 Comparison

Device	Responsivity	I _{ph} /I _{dark}	Detectivity
Perovskite Based [This device]	0.45 A/W	9.16×10^6	6.01×10^{11} Jones
ZnO/Polymer based [24]	0.18A/W	10000	-
Perovskite/Conjugated-Polymer Composite[25]	0.154 A/W	-	8.8×10^{10} Jones
Organic Bulk Heterojunction [23]	0.11 A/W	-	3.15×10^{11} Jones

IV. CONCLUSION

Simulation analysis of a CH₃NH₃PbI₃-xCl_x based perovskite device as a solar cell and photodetector has been performed in this work. High optical absorption coefficient, large diffusion lengths of carriers and wide spectral response of perovskite

material make the device suitable for solar cell and photodetector applications. As a solar cell the device shows high open circuit voltage and high power conversion efficiency. Various parameters of the solar cell have been optimized to maximize the performance of the solar cell. It is shown that the thickness of the perovskite absorber and the choice of electrode material greatly affect the performance of the perovskite device. Combination of FTO as front electrode and gold as back electrode is found to be best for the device performance. The maximum power conversion efficiency is achieved at a perovskite absorber thickness of 2.3 μm . At this thickness the perovskite solar cell offers a maximum power conversion efficiency of 22.7% and an open circuit voltage of 1.13V. The simulation of perovskite device as a photodetector shows that it offers a high responsivity over a large wavelength range and a high detectivity. At 600 nm incident light wavelength it achieves a maximum responsivity of 0.45 A/W and a detectivity of 6.01×10^{11} Jones for an optimum perovskite absorber thickness of 500 nm. The high values of responsivity and detectivity and the simplicity of device structure make the device promising candidate for photodetector applications. The role of device parameters like thickness, doping concentration and defect density of perovskite absorber on the photodetector performance was also investigated. It is hoped that this work would help to further advance the development of perovskite based photovoltaic devices.

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