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# EFFECT OF N-TYPE TRANSITION METAL DICHALCOGENIDE MOLYBDENUM TELLURIDE (N-$MoTe_2$) IN BACK CONTACT INTERFACE OF CADMIUM TELLURIDE SOLAR CELLS FROM NUMERICAL ANALYSIS

N. DHAR[a], T. H. CHOWDHURY[a], M. A. ISLAM[a], N. A. KHAN[a], M. J. RASHID[a], M. M. ALAM[c], Z. A. ALOTHMAN[c], K. SOPIAN[a], N. AMIN[a,b,c*].

[a]*Solar Energy Research Institute (SERI), Universiti Kebangsaan Malaysia, 43600, Bangi, Malaysia*

[b]*Faculty of Engineering and Built Environment, Universiti Kebangsaan Malaysia, 43600, Bangi, Malaysia*

[c]*Advanced Materials Research Chair, Chemistry Department, College of Sciences, King Saud University, Riyadh 11451, Saudi Arabia*

The effects of unintentionally formed n-type transition metal dichalcogenide namely molybdenum telluride ($MoTe_2$) in between Cadmium Telluride (CdTe) absorber layer and Mo back contact is studied from numerical modeling and analysis. The main objective is to analyze the possible effects of n-$MoTe_2$ formation in CdTe thin film solar cell. Energy band line-up of Mo/$MoTe_2$/CdTe interface is investigated in order to explain the interface properties with different parameters. Carrier concentration, bandgap energy, electron affinity and thickness of n-$MoTe_2$ have been varied in the numerical simulation to observe its effects on overall photovoltaic performance. The increase in the carrier concentration and bandgap energy of n-$MoTe_2$ deteriorates the overall performance. This could be attributed to the high value of built-in-potential ($V_{bi}$) along with band offset value at n-$MoTe_2$/p-CdTe interface, which causes the electrons to be drifted back towards the back contact and results in recombination. Advantageous effects are observed as the electron affinity of n-$MoTe_2$ is increased. This can be explained by the lower value of band offset ($\Delta E_C$ and $\Delta E_V$) at n-$MoTe_2$/p-CdTe interface that interrupts the flow of carriers in overall circuit in a moderate way. Numerical results reveal that n-$MoTe_2$ layer thinner than 50 nm affects adversely, possibly due to the shunting.

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*Keywords:* Thin film solar cells, CdTe, Substrate configuration, $MoTe_2$

## 1. Introduction

Cadmium Telluride (CdTe) based solar cell, as shown in Fig. 1, is one of the promising candidates due to its high efficiency and low cost potentials among the thin film groups. Up to date, the highest attained efficiency in case of CdTe solar cell is about 20.4% [1]. Besides, amongst thin film solar cells, CdTe has the largest PV industrial production with lowest cost of USD 0.75, while the module efficiency was about 11% [2, 3]. However, due to its high work function (5.79 eV), it is quite hard to find an appropriate metal as back contact. Most of the high efficiency reported until now are using some pseudo contact layers between the back contact layer and CdTe absorber layer [4-7]. Hence, molybdenum (Mo) is a prominent back contact for CdTe thin film solar cell with work function of 4.6 eV [8]. In comparison with other back contacts (for example gold, platinum), Mo is low cost as well as more available. Formation of ohmic back contact is very much important in order to reduce the series resistance for solar cells. As found from other studies related to CIGS, unintentionally formed transition metal dichalcogenide, p-

*Corresponding author: nowshad@eng.ukm.my

$MoSe_2$ in between the CIGS and Mo interface reduces the series resistance as well as enhances the overall performance for CIGS solar cells. However, for CdTe solar cells instead of p-$MoSe_2$, p-$MoTe_2$ or n-$MoTe_2$ may form at the interface of Mo and CdTe that may have a major impact on overall cell performance.

In this study, we demonstrate the possible effects of unintentionally formed transition metal dichalcogenide, n-$MoTe_2$ layer in between the CdTe absorber layer and Mo back contact from theoretical approach along with numerical modeling.

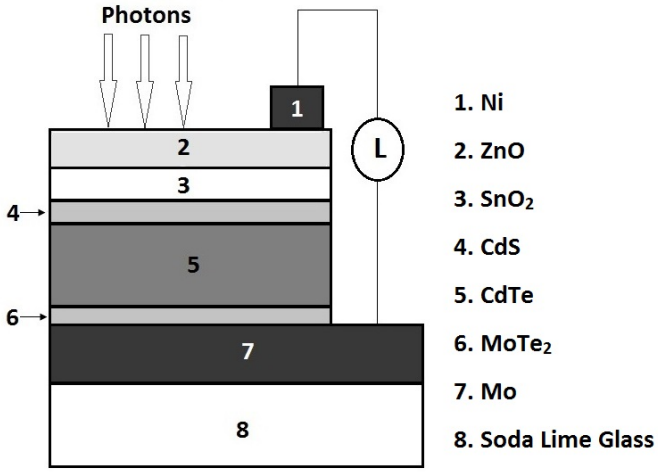


*Fig. 1: Schematic diagram of CdTe solar cell with $MoTe_2$ layer*

## 2. Methodology

### 2.1 Device simulation

In this numerical study, AMPS-1D software is used to analyze the effects of unintentionally formed $MoTe_2$ layer in CdTe thin film solar cell. By introducing the various material parameters into AMPS-1D software (as given in Table 1) for all sorts of possible analysis aspects, effects on the values of efficiency, $J_{sc}$, $V_{oc}$ and FF of are observed [9-16]. In this study, we have investigated the effects of unintentionally formed n-type $MoTe_2$ at the back contact as the worst case scenario. The carrier concentration and the electron affinity of n-$MoTe_2$ is have been changed from $1\times10^{13}$ to $1\times10^{17}$ $cm^{-3}$ and 3.8 to 4.2 eV, while the energy bandgap and the thickness of n-$MoTe_2$ layer varied from 0.91 to 1.1 eV and from 10 to 100 nm, respectively, in order to observe its effect on the overall performance of the CdTe solar cells.

*Table 1. Material Properties used in Numerical Analysis*

| Property | $SnO_2$ | $Zn_2SO_4$ | CdS | CdTe | $MoTe_2$ |
|---|---|---|---|---|---|
| Thickness (μm) | 0.07 | 0.1 | 0.08 | 2 | 0.01-0.1 |
| $\varepsilon_r$ | 9 | 9 | 9 | 9.4 | 13 |
| $\mu_n$ ($cm^2 V^{-1} s^{-1}$) | 100 | 32 | 350 | 320 | 110 |
| $\mu_p$ ($cm^2 V^{-1} s^{-1}$) | 25 | 3 | 50 | 40 | 426 |
| $N_A$ ($cm^{-3}$) | 0 | 0 | 0 | $5\times10^{16}$ | 0 |
| $N_D$ ($cm^{-3}$) | $10^{17}$ | $10^{17}$ | $10^{19}$ | 0 | $4\times10^{13}$-$4\times10^{18}$ |
| $E_G$ (eV) | 3.6 | 3.35 | 2.42 | 1.45 | 0.91-1.1 |
| $N_C$ ($cm^{-3}$) | $2.2\times10^{18}$ | $2.2\times10^{18}$ | $2.2\times10^{18}$ | $7.5\times10^{17}$ | $3\times10^{18}$ |
| $N_V$ ($cm^{-3}$) | $1.8\times10^{19}$ | $1.8\times10^{19}$ | $1.8\times10^{19}$ | $1.8\times10^{19}$ | $4\times10^{18}$ |
| $\chi$ (eV) | 4.5 | 4.5 | 4.5 | 4.28 | 3.8-4.2 |

### 2.2 Theoretical analysis

As $MoTe_2$ is a semiconducting material, it can be either n-type or p-type. The interface properties of Mo/$MoTe_2$/CdTe strongly depend on the conductivity type of $MoTe_2$. The Mo/$MoTe_2$ metal-semiconductor interface can be either an ohmic type or a rectifying type, precisely depending on the metal ($\Phi_m$) and semiconductor work functions ($\Phi_s$). The difference between the values of semiconductor and metal work function potentials is commonly known as Equilibrium contact potential ($V_0$).The equilibrium contact potential ($V_0$), which forms in between Mo and $MoTe_2$ is also assumed to be influenced by the various types of conductivity of $MoTe_2$ layer. This is due to the dependency of $\Phi_s$ to the doping level ($N_D$ or $N_A$) as well as conductivity type (n or p) of the semiconductor material itself. In case of a metal and n-type (or p-type) semiconductor junction, diffusion of electrons (or holes) is prevented by $V_0$ from the semiconductor side to the metal side. From the hetero-junction formation point of view it can be said that, p-type $MoTe_2$ forms isotype hetero-junction while n-type $MoTe_2$ will forms aniso-type hetero-junction with p-CdTe absorber layer. Here, conduction band offset ($\Delta E_c$) and valence band offset ($\Delta E_v$) for both n-$MoTe_2$/CdTe and p-$MoTe_2$/CdTe are similar in values as long as electron affinity and energy bandgap are not dependent on the doping profile. Fig. 2 shows the possible Mo/$MoTe_2$/CdTe interface configurations that might take place.

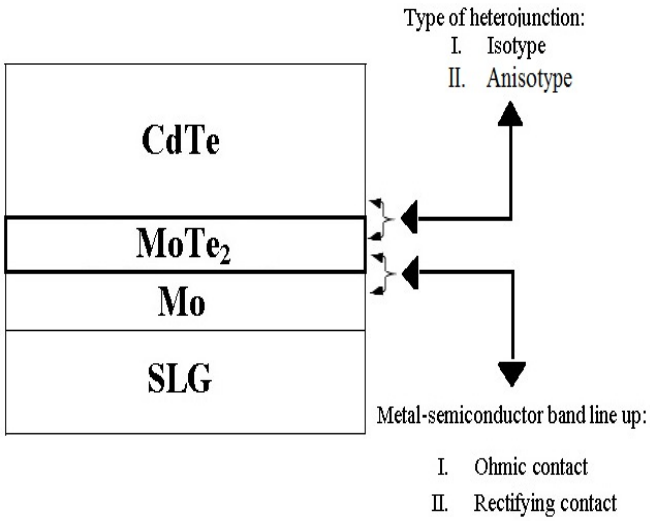


*Fig. 2: Schematic diagram of Mo/$MoTe_2$/CdTe interfaces*

## 3. Results and Discussion

The band profile of Mo/$MoTe_2$/CdTe structure as shown in Fig. 3 is analyzed in order to reveal the metal-semiconductor-semiconductor properties. The type of contacts for both Mo/n-$MoTe_2$ and Mo/p-$MoTe_2$ structures as shown in Table 2 are found to be highly effected with the variation in $MoTe_2$ doping level (degenerate is assumed). This is because, the Fermi level of Mo ($E_{Fm}$) lies in between the energy band structure of $MoTe_2$. Hence, n-$MoTe_2$ may forms ohmic contact or rectifying contact with Mo depending upon the doping level of $MoTe_2$. While the contact formation between p-$MoTe_2$ and Mo is always rectifying in nature. However, the equilibrium contact potential ($V_0$) which inhibits the diffusion of hole into metal in Mo/p-$MoTe_2$ structure decreases as the doping level ($N_A$) in being lowered. Lower doping level causes the Fermi level to be shifted upwards.

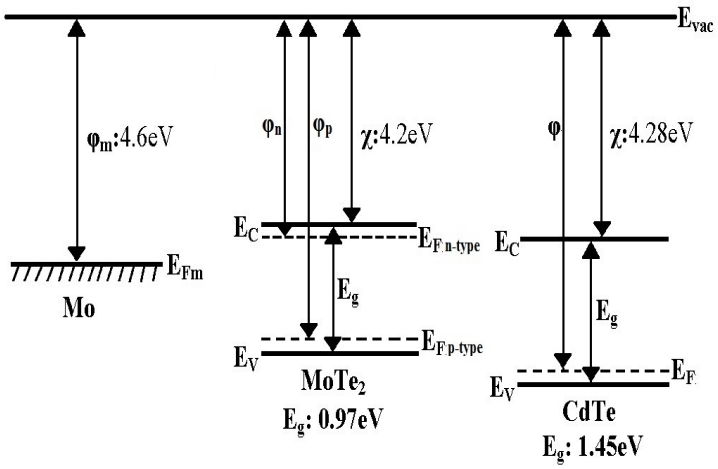


*Fig. 3: Energy band diagrams of Mo, $MoTe_2$ and CdTe in isolation*

Hence, due to this semiconductor work function potential and subsequently, $V_0$ decreases. In overall it can be deduced that, the interface properties p-$MoTe_2$ in CdTe solar cell is similar to the interface properties of p-$MoSe_2$ in CIGS solar cell. The contact formation of p-$MoTe_2$ with Mo in CdTe solar cell is rectifying in nature, which is exact similar to the p-$MoSe_2$ in CIGS solar cell. It should not be confound with the fact that p-$MoSe_2$ makes an ohmic contact with CIGS absorber layer, not with Mo back contact.

Undesirable effect is noticed in the photocurrent collection for CdTe solar cells with n-$MoTe_2$ layer for the doping level of $1\times10^{18}$ $cm^{-3}$. Fig. 4 exhibits the performance parameters of CdTe solar cells with various n-$MoTe_2$ carrier concentrations.

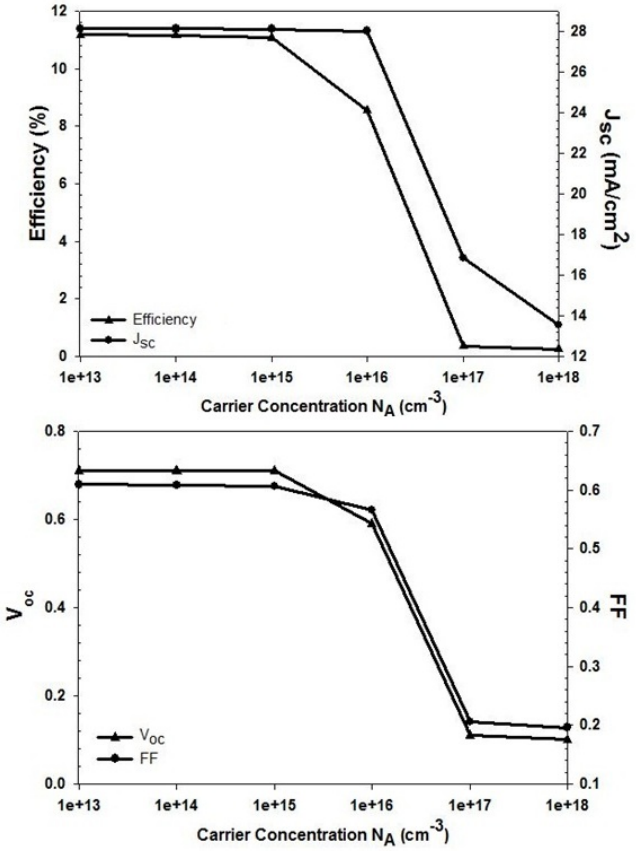


*Fig. 4: CdTe performance parameters with different n-$MoTe_2$ carrier concentration*

Variation in the carrier concentrations of n-$MoTe_2$ affects both of Mo/n-$MoTe_2$ and n-$MoTe_2$/p-CdTe interface properties. As mentioned earlier, while the carrier concentration of n-$MoTe_2$ increases, the Fermi level shifts upwards that is closer to the conduction band edge. Hence, this phenomenon causes the semiconductor work function potential to be decreased. The contact type of n-$MoTe_2$ with Mo highly depends upon the doping level of n-$MoTe_2$. For high doping level, n-$MoTe_2$ forms schottky contact with Mo which can be advantageous for the solar cell (possibly due to less recombination). However, increasing the doping level of n-$MoTe_2$ causes the built in potential ($V_{bi}$) at n-$MoTe_2$/p-CdTe interface to be increased, while $V_{bi}$ of the semiconductor interface diode is directly proportional to the carrier concentration at both side of the semiconductor in a p-n junction. Due to this additional built in potential, electrons that are photo generated in the vicinity of n-$MoTe_2$/p-CdTe interface will be drifted back to the back contact. Hence, the carriers will move in the opposite direction in which they move in conventional solar cells. However, the carriers will be hindered while moving through Mo/n-$MoTe_2$ interface as the contact is Schottkty type. Thereby, this phenomenon tends to increase the recombination rate at the back contact diode. Besides, at the same time holes will repel to the front contact, which will result in the net photo-generated current to be decreased. Hence, this is consistent with the results from this numerical study. It was observed that, when as the carrier concentration is increased $1\times10^{16}$ to $1\times10^{18}$ $cm^{-3}$ $J_{sc}$ drops almost 51.84 %. Besides, solar cell performance parameters like as $V_{oc}$, FF as well as efficiency decrease drastically as doping level of n-$MoTe_2$ increases from $10^{16}$ to $10^{17}$ $cm^{-3}$ (Fig. 4). On the other hand, as the doping level n-$MoTe_2$ decreases, it gradually forms ohmic contact with Mo, which can be detrimental to overall solar cell performance by increasing the recombination rate at the back contact diode. By lowering the doping level of n-$MoTe_2$, the built-in-potential at n-$MoTe_2$/p-CdTe interface also decreases. Therefore, the probability of photo-generated electrons which are drifted back to the back contact by the additional built in potential ($V_{bi}$) will be minimized. Hence, overall solar cell performance is improved. This observation implies that the unfavorable Mo/n-$MoTe_2$ interface property due to the increase in n-$MoTe_2$ carrier concentration is somehow offset by the favorable changes in n-$MoTe_2$/p-CdTe interface. Solar cell performance parameters like as $V_{oc}$, $I_{sc}$, FF as well as efficiency improves as doping level of n-$MoTe_2$ decreases. Hence, it can be concluded that doping level of n-$MoTe_2$ is inversely proportional to solar cell performance parameters from this numerical study.

*Table 2. Mo/$MoTe_2$/CdTe interface properties.*

| $MoTe_2$ | Mo-$MoTe_2$ contact type (Ohmic) | Mo-$MoTe_2$ contact type (Rectifying) |
|---|---|---|
| p-type | $\Phi_{Mo} > \Phi_p$ | $\Phi_{Mo} < \Phi_p$ |
| n-type | $\Phi_{Mo} < \Phi_n$ | $\Phi_{Mo} > \Phi_p$ |

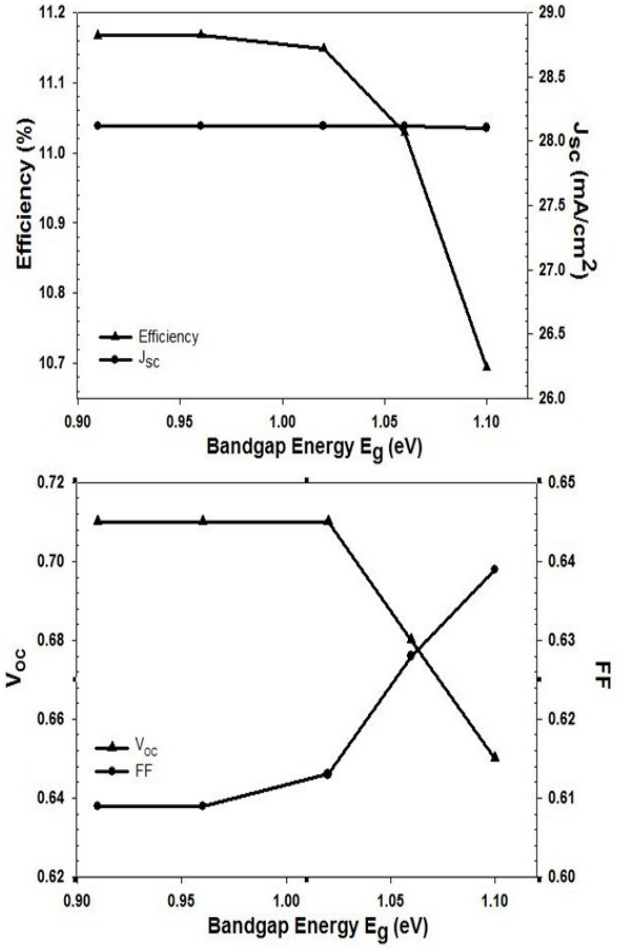


*Fig. 5: CdTe performance parameters with different n-$MoTe_2$ Band gap energy*

On the variations in the bandgap energy of n-$MoTe_2$, even a small increment (<0.2 eV) the CdTe solar cell conversion efficiency degrades (Fig. 5). An increase in the bandgap energy value, that is from 0.91 eV to 1.1 eV causes the conversion efficiency to be decreased. Increment in the n-$MoTe_2$ bandgap (Possibly due to downward shift of $E_v$ as well as upward shift of $E_c$) decreases the electron affinity. As a result, the value of conduction band offset ($\Delta E_c$) increases and valance band offset ($\Delta E_v$) decreases. In general, the value of $\Delta E_c$ at n-$MoTe_2$/p-CdTe junction is a lower value (< 0.1 eV), While the value of $\Delta E_v$ is quite high (> 0.6). Table 3 shows the possible values of band offset at n-$MoTe_2$/p-CdTe junction on the variation of $MoTe_2$ bandgap energy.
The equations used to calculate the values of $\Delta E_c$ and $\Delta E_v$ are given below,

$$\Delta E_c = \chi_{CdTe} - \chi_{MoTe_2} \tag{1}$$

$$\Delta E_v = (\chi + E_g)_{CdTe} - (\chi + E_g)_{MoTe_2} \tag{2}$$

Here, $E_g$ is energy and $\chi$ is electron affinity bandgap in both equation (1) and (2). As the bandgap energy value of n-$MoTe_2$ is increasing (Possibly due to downward shift of $E_v$ and upward shift of $E_c$), $\Delta E_v$ is decreasing, though the value is still high (> 0.49 eV) for holes to transport towards n-$MoTe_2$. Besides, $\Delta E_c$ now becomes higher in value (> 0.19 eV) than before. Therefore, electrons which were drifted towards n-$MoTe_2$/p-CdTe interface with greater ease, now slightly impeded by larger value of $\Delta E_c$ (> 0.19 eV). While, hole transport is still impeded by larger value of $\Delta E_v$ (> 0.49 eV). As a result, overall cell performance decreases as shown in Fig. 5.

*Table 3 Barrier height and band offset for Mo/n-$MoTe_2$ and n-$MoTe_2$/p-CdTe interface*

| Metal work function ($\varphi_M$) (eV) | Hetero-junction Type | Electron Affinity ($\chi$) (eV) | Barrier Height ($\varphi_{BP}$)at Mo/n-$MoTe_2$ Interface (eV) | $\Delta E_C$ at n-$MoTe_2$/p-CdTe interface (eV) | $\Delta E_V$ at n-$MoTe_2$/p-CdTe interface (eV) |
|---|---|---|---|---|---|
| | | 3.8 | 0.8 | 0.48 | 0.91 |
| | | 3.85 | 0.75 | 0.43 | 0.86 |
| | | 3.9 | 0.7 | 0.38 | 0.81 |
| | | 3.95 | 0.65 | 0.33 | 0.76 |
| 4.6 | Anisotype | 4 | 0.6 | 0.28 | 0.71 |
| | | 4.05 | 0.55 | 0.23 | 0.66 |
| | | 4.1 | 0.5 | 0.18 | 0.61 |
| | | 4.15 | 0.45 | 0.13 | 0.56 |
| | | 4.2 | 0.4 | 0.08 | 0.51 |

The overall cell performance varies at the variation of electron affinity as shown in Fig. 6. Positive effect was observed while electron affinity increases and performance deteriorates as electron affinity decreases.

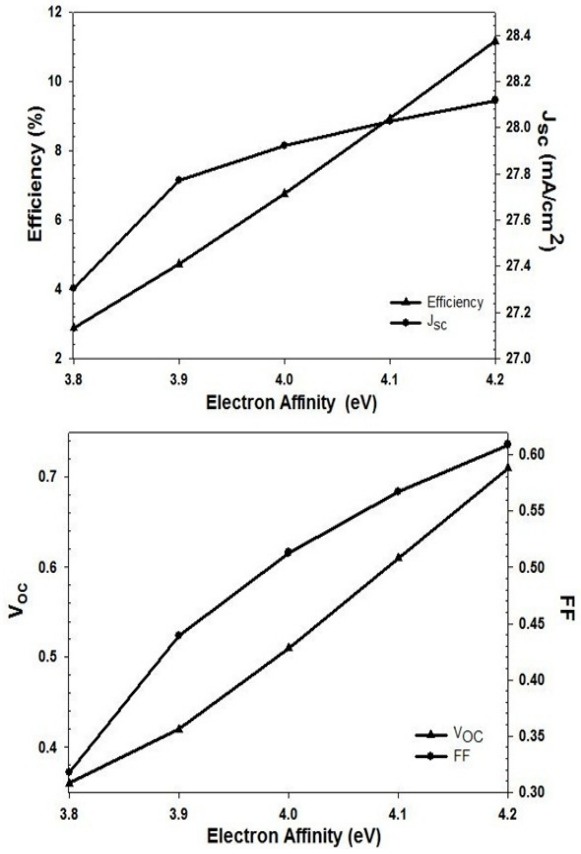


*Fig. 6: CdTe performance parameter with different n-MoTe2 electron affinity*

It is well known that as the electro affinity decreases both the conduction band and the valance band move upward and vice versa. It is clear from the Fig. 3 that conduction band and valance band of CdTe take position below the conduction and valance band of $MoTe_2$, respectively. Hence, as the electron affinity decreases the conduction band offset ($\Delta E_c$) and valance band offset ($\Delta E_v$) at n-$MoTe_2$/p-CdTe junction increase. Consequently, both holes and electrons face a higher barrier height while moving to their respective direction. This barrier

compels the electrons and holes to drift back to the opposite direction in comparison to the direction in the conventional solar cell. Additionally, the barrier height ($\varphi_{Bp}$) at Mo/n-$MoTe_2$ junction, which intends to prevent the flow of electron from n-$MoTe_2$ to back contact, also increases as the electron affinity decreases. The possible values of barrier height ($\varphi_{Bp}$) on the variation of electron affinity have given in Table 3. Besides, due to the decrease in electron affinity of n-$MoTe_2$, the built in potential ($V_{bi}$) at n-$MoTe_2$/p-CdTe interface and equilibrium contact potential ($V_0$) at Mo/n-$MoTe_2$ interface are also to be increased. Hence, the effect of the higher value of $V_0$ which is beneficial for solar cell performance by preventing the backward flow of electron is somehow offset by the higher value of $V_{bi}$. These factors enhance the electron recombination mechanism at the back contact. Therefore, photocurrent loss increases which is manifested by the decreasing $J_{sc}$ values as n-$MoTe_2$ electron affinity values decreases from 4.2 eV to 3.8 eV. As a result, overall solar cell performance becomes worse. A decrease of 9.52% in the electron affinity results in 74.17% decrease in conversion efficiency. On the contrary, solar cell performance parameter parameters such as $V_{oc}$, $J_{sc}$, FF as well as efficiency improve as the electron affinity increases. This could be due to the lower value of band offset ($\Delta E_c$ and $\Delta E_v$) as well as lower value of $V_{bi}$ at n-$MoTe_2$/p-CdTe interface. By increasing the electron affinity, $V_0$ at Mo/n-$MoTe_2$ interface decreases, which helps to reduce the recombination rate by preventing the flow of electron to the back contact. However, this unfavorable effect is somehow offset by the favorable effect of the lower value of $V_{bi}$ at n-$MoTe_2$/p-CdTe interface and consequently, solar cell performance improves.

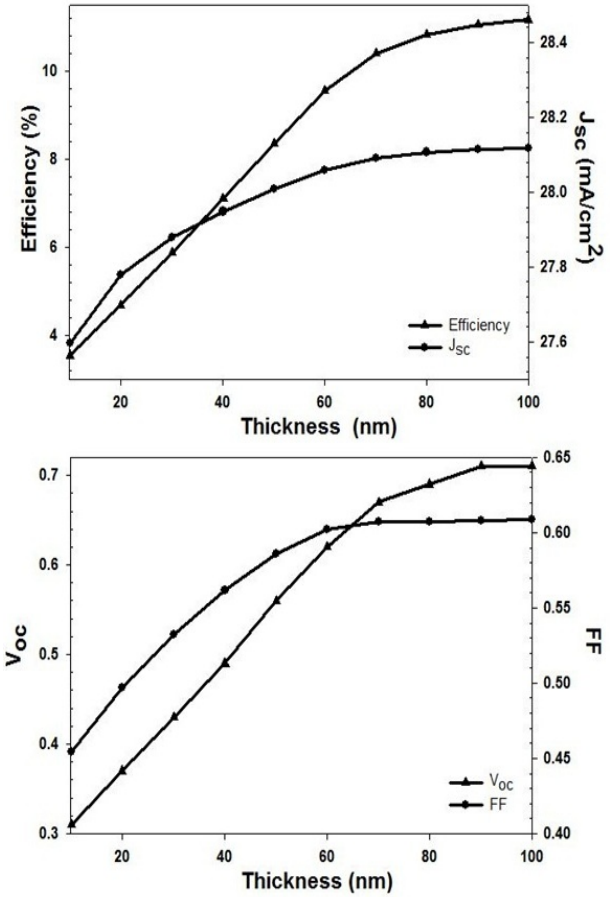


*Fig. 7. CdTe performance parameter with different n-$MoTe_2$ thickness.*

From the numerical study as shown in the Fig. 7 it is found that $MoTe_2$ ($E_g$=0.97 eV) layer thinner than 50 nm is detrimental for overall CdTe solar cell performance. This is because n-$MoTe_2$ layer with low thickness causes lower shunt resistance that is evident from the lower value of $V_{oc}$. Hence, depend upon the numerical results from this it is very likely that, n type $MoTe_2$ layer with appreciable thickness forms in between Mo back contact and p-CdTe absorber layer.

## 4. Conclusion

In this study, the effects of unintentionally formed n-$MoTe_2$ layer in between CdTe absorber layer and Mo back contact is studied from numerical analysis. The results form numerical modeling show that n-$MoTe_2$ layer has some undesirable effect on the CdTe solar cell performance due to the unfavorable band line-up properties of Mo/n-$MoTe_2$ and n-$MoTe_2$/p-CdTe interfaces. Adverse effect is also observed as carrier concentration and bandgap energy value of n-$MoTe_2$ increases. This is due to the high built-in-potential ($V_{bi}$) and band offset ($\Delta E_C$ and $\Delta E_V$), which eventually cause higher recombination rate. Decreasing the electron affinity of n-$MoTe_2$ decreases the short circuit current ($J_{sc}$) values by increasing the photocurrent loss. As a result, overall cell performance deteriorates. Thinner n-$MoTe_2$ (< 50 nm) also decreases the overall conversion efficiency.

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