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Design modern structure for heterojunction quantum dot solar cells

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Article Info

ABSTRACT

This paper proposal new structure for improving the optical, electrical characteristics and efficiency of 3rd generation heterojunction quantum dot solar cell (HJQDSC) (ITO/CdS/QDPbS/Au) model by using the quantum dot window layer instead of bulk structure layers cell. Also, this paper presents theoretically analysis for the performance of the proposal HJQDSC (ITO/QDCdS/QDPbS/Au) structure. The new design structure was applied on traditional (SnO2/CdS/CdTe/Cu) and (ZnO/CdS/CIGS/Mo) thin film solar cells which based on sub-micro absorber layer thickness models by replacing the bulk CdTe, CIGS absorber layers and CdS window layer with quantum dot size materials to achieve higher efficiency with lesser usage layer material. Also, it has been studied the effect of using semiconductors layers in quantum dots size on electric and optical properties of thin film solar cells and the effect of window and absorber layers quantum dots radii on the performance of solar cells. Finally, a thermal efficiency analysis has been investigated for explaining the importance of new structure HJQD solar cells.

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1. INTRODUCTION

Several solar technologies including wafer, thin film and organic, have been researched to achieve reliability, cost-effectiveness and high efficiency. Cost effectiveness can be seen in the use of less material as well as increasing energy conversion efficiency. The reduction in the efficiencies of the previous models due to the reduction of absorber layers thickness are associated with a number of problems [1-3]. The 3rd generation of solar cells technique based on novel absorber layer materials with tunable bandgap that can be tuned to match the spectral distribution of solar spectrum are crucial and achieved less consummation absorber layer material. Quantum dots have the merit of tunable bandgap as a result of size variation as well as formation of intermediate bands. The energy band gap increases with a decrease in size of the quantum dot, the adjustable bandgap of quantum dots allows the construction of nanostructured solar cell that is able to harvest more of the solar spectrum [4]. Quantum dots can generate multiple exciton (electron-hole pairs) after collision with one photon of energy exceeding the band gap. Absorption of UV photons in quantum dots produces more electrons than near infrared photons. Quantum dots emit up to three electrons per photon due to multiple exciton generation as opposed to only one for standard crystalline silicon solar cell [5]. The previous study for heterojunction solar cells based on PbS-QDs/CdS thin films demonstrating an achieved efficiency of 3.3% [6].

This paper proposal new structure for previous heterojunction quantum dot ITO/CdS/QDPbS/Au thin film solar cell model to improve the efficiency of the model by using the quantum dot absorber layer and replaced the bulk CdS window layer with quantum dot CdS layer. It has been applied the new structure model on the previous SnO$_2$/CdS/CdTe/Cu and ZnO/CdS/CIGS/Mo thin film models which based on sub-micro absorber layer thickness to improve the performance and efficiency of the cells to save the consumption in the absorber layer material. The effect of window and absorber layers' quantum dots radii on the performance of the selected cells. A comparative study is done for specifying the best size of window and absorber layer materials to achieve higher efficiency with lesser usage semiconductor materials and lesser production cost and time.

2.   MATHEMATICAL MODELS OF PROPOSAL HJQD THIN FILM SOLAR CELLS

Considering spherical shape of nanostructure layer material in thin film solar cell, based on the model developed by Louis Brus for colloidal quantum dots. The energy band gap of quantum dot layer material can be approximated by 1, and that bandgap energy values increase as the quantum dot size decreases [7].

$$E_{g(Qdots)} = E_{gbulk} + \frac{\pi^2 h^2}{2R^2}\left(\frac{1}{m_{eb}} + \frac{1}{m_{hb}}\right) - \frac{1.8Q^2}{4\pi\varepsilon_b\varepsilon_o R} \tag{1}$$

where: R is radius of quantum dot layer material, m_{eb}, m_{hb} are the effective mass of electron and hole for layer material, Q is the elementary charge, ε_0 is the permittivity of free space, and h is Plank constant. The energy bandgap value of the bulk layer material calculated using Varshni relation temperature dependence of the bandgap in semiconductors which using in absorber or window layer can be described as [8-10].

$$E_{gbulk} = E_g(0) - \frac{\varsigma T^2}{\beta} \tag{2}$$

where, $E_g(0)$ is energy band gap of semiconductor material at zero temperature, ς and β are constants, ε_b is dielectric constant of the semiconductor layer material which can be described by using the Drude model [11-12] as follows:

$$\varepsilon_b = \varepsilon_{b\infty}\left(1 - \frac{\omega_b^2}{\omega^2 + i\omega(\gamma_{mb})}\right) \tag{3}$$

where, ω is angular frequency of light, ω_0 is the plasma angular frequency of semiconductor layer material, γ_{mb} is the damping frequency of semiconductor layer material. Whatever, $\varepsilon_{b\infty}$ is the infinity dielectric constantof semiconductor layer materials that can be determined as follows:

$$\varepsilon_{b\infty} = \varepsilon_o\left(1 + \frac{\omega_b^2}{(E_{gbulk})^2}\right) \tag{4}$$

Also, G_{QD} is the electron–hole pair generation rate in the quantum dot absorber layer can be written with the aid of the following [13]:

$$G_{QD}(\lambda) = \frac{\alpha_{bQD}(\lambda)e^{-\alpha_{wQD}(d_w)}[1 - R_{QD}(\lambda)]\lambda I_o(\lambda)}{hc} \tag{5}$$

where, λ is the photon wavelength, $\alpha_{wQD}d_w$ is the absorption coefficient and thickness of the thin top semiconductor layer (n-layer CdS), α_{bQD} is the absorption coefficient of the absorber layer (CdTe, GIGS or PbS), $R_{QD}(\lambda)$ is reflection of front layer material (SnO$_2$, ZnO or ITO), and $I_o(\lambda)$ is the intensity of the solar spectral, c is the speed of light. The absorption coefficient of the absorber and window quantum dots layers ($\alpha_{bQD}(\lambda)$ and α_{wQD}) can be calculated based on the Beer-Lambert's law as follows [14]:

$$\alpha_{QD}(\lambda) = \frac{2.303 \times A_{tQD}}{d_t} \tag{6}$$

where, A_{tQD} is the absorbance of the absorber or window layer that calculated as follows:

$$A_{tQD} = 1 - T_{tefQD} - R_{tefQD} \tag{7}$$

also, R_{tefQD} and T_{tefQD} are the reflectance and transmittance of quantum dot window or absorber layer that evaluated from the following [15]:

$$R_{tefQD} = \frac{P_{QD}^2 + Z_{QD}^2 + 2P_{QD}Z_{QD}cos\theta}{1 + 2P_{QD}^2 Z_{QD}^2 + 2P_{QD}Z_{QD}cos\theta}, \text{ and } T_{tefQD} = \frac{16n_0^2 n_{tQD}^2 n_s}{1 + 2P_{QD}^2 Z_{QD}^2 + 2P_{QD}Z_{QD}cos\theta} \tag{8}$$

The refractive index or substrate of quantum dot thin film material (n_{tQD}, n_{sQD}) window or absorber layer has been calculated as follows:

$$n_{bQD} = \sqrt{\frac{|\varepsilon_{bQD}| + \varepsilon_{rebQD}}{2}} \tag{9}$$

The dielectric constant of the quantum dot semiconductor layer material, which can be described by using the Drude model with respect to [11, 12, 16, 17] as follows:

$$\varepsilon_{bQD} = \varepsilon_{b\infty QD}\left(1 - \frac{\omega_b^2}{\omega^2 + i\omega(\gamma_a)}\right), \text{ and } \varepsilon_{b\infty QD} = \varepsilon_o\left(1 + \frac{\omega_b^2}{\left(E_{g(Qdots)}\right)^2}\right) \tag{10}$$

The refractive index of front thin film layer material (ZnO, ITO or SnO₂) n_x calculated using sellmeier equations [18, 19]. The substrate layer material of absorber layer is metallic material (Cu, Au, Mo). The dielectric constant of the metallic material ε_m can be described as [16]:

$$\varepsilon_m = \varepsilon_{INTRA} + 1 - \frac{\omega_m^2}{\omega^2 + i\omega(\gamma_m)} \tag{11}$$

where, γ_m is the macroscopic damping constant due to the dispersion of the electrons by the ions of the system of metallic, ω_m is the plasma angular frequency, ε_{INTRA} is the contribution from the intra-band transitions. The refractive index of substrate layer material of absorber layer calculated using the dielectric constant of metallic substrate layer ε_m the forward diode current of proposal heterojunction quantum dot cells can evaluate [13] as:

$$J_{diQD}(V) = J_{OQD}\left[exp\left(\frac{Q(V + J(V)R_{ser})}{nKT}\right) - 1\right] \tag{12}$$

$$J_{OQD} = \frac{W_{QD}Q\sqrt{N_{con}N_{val}exp\left(-\frac{E_{gbQD}}{KT}\right)}}{\sqrt{\dagger_e\dagger_h}} \tag{13}$$

where, J_{OQD} is reverse saturation current density in quantum dot cells, n is the diode quality factor, R_{ser} is series resistance. The width of the depletion layer depends on the dielectric constant of quantum dot absorber layer material ε_{bQD} that can be calculated by the following expression [20].

$$W_{QD} = \sqrt{\frac{2\varepsilon_0\varepsilon_{bQD}(V_{bi} - V)}{Q(N_a - N_d)}} \tag{14}$$

where V_{bi} is the built-in potential, $N_a - N_d$ is the concentration of uncompensated acceptors. Whatever, total photo generated current density, the open circuit voltage, efficiency and fill factor of proposal heterojunction quantum dot models can be obtained [13] as:

$$J_{phQD}(V) = \int_0^\infty J_{TQD}(\lambda.V)d\lambda \tag{15}$$

The resultant photocurrent density $J_{TQD}(\lambda.V)$ dependent on the generation rate and depletion width of heterojunction quantum dot cell based on [13]. The net external current density from proposal heterojunction quantum dot a solar cell obtained by the following expression [21]:

$$V = J_{phQD}(V) - J_{diQD}(V) - \left(\frac{V + J(V)R_{ser}}{R_{sh}}\right) \tag{16}$$

where, R_{sh} is the shunt resistance, V is the applied voltage. Moreover, the open circuit voltage of quantum dot thin film solar equation is expressed as follows [22]:

$$V_{ocQD} = \left(\frac{KT}{Q}\right) \ln\left[\frac{J_{phQD}}{J_{OQD}} + 1\right] \tag{17}$$

$$P_{QD} = J \times V \tag{18}$$

where: P_{maxQD} is the maximum point of output power density of quantum dot cell which calculate from $P_{QD} - V$ curve. Final form of efficiency and Fill factor of quantum dot thin film solar cell calculated by the following expression [22]:

$$F.FQD = \frac{P_{maxQD}}{V_{ocQD} \times J_{phQD}} \tag{19}$$

$$n_{QD} = \frac{J_{phQD} V_{ocQD} F.FQD}{P_{in}} \times 100 \tag{20}$$

3. QUANTUM SOLAR CELLS PARAMETERS

The proposal models are used parameters of traditional practical models by using new techniques, thus, it has been achieved new high efficiency quantum dot solar cells with smallest absorber and window layer thickness for saving the consumation of materials and hence reducing the cost [2, 3, 6]. Tables 1-3 depicts the main parameters of proposal heterojunction quantum dot thin film models.

Table 1. Parameters of usage substrate materials for absorber layer [23-25]

Materials	Plasma angular frequency ($\omega_p 10^{16}$rad/s)	Damping constant ($\gamma_m\ 10^{13}$ s^{-1})
Cupper (Cu)	1.03	5.26
Gold (Au)	1.29	0.549
Molybdenum	0.19	1.14

Table 2. Parameters of usage materials [2, 3, 6, 26]

Parameters	CdTe	CIGS	PbS	CdS
Bulk energy band gap (eV) at room temperature	1.5	1.10	0.395	2.40
Bulk absorption coefficient $\times 10^5$Cm^{-1}	0.4	0.50	0.008	0.9
Absolute bulk dielectric constant	9.5	13.6	18.6	10.2
Band gap (eV) at zero Kelvin	1.6077	1.25	0.543	2.58
Band gap parameter G (eVK^{-1}) $\times 10^{-4}$	3.1	1.02	5	4.202
Band gap parameter β (K)	108	272	0.40	147
Electron mobility (Cm^2/Vs)	320	100	1000	350
Hole mobility (Cm^2/Vs)	40	25	80	50
Effective mass of electron	0.11	0.09	0.1	0.2
Effective mass of holes	0.35	0.75	0.1	0.7
Plasma angular frequency ($\omega_p \times 10^{16}$rad/s)	0.052	0.039	0.014	0.082
Damping constant ($\gamma_m \times 10^{13}$ s^{-1})	8.88	19.5	1.76	17.6
Fermi velocity ($v_f \times 10^6$ m/s)	0.59	0.45	8	0.89

Table 3. Parameters of usage thin film solar cells models [2, 3, 6]

Parameters	SnO$_2$/CdS/CdTe/Cu	ZnO/CdS/CIGS/Mo	ITO/CdS/QDPbS/Au
Absorber layer thickness (nm)	500	360	200
Window layer thickness (nm)	100	40	70
Front layer thickness (nm)	100	450	100
Electron lifetime (s)	1×10^{-8}	16×10^{-7}	16×10^{-5}
Hole lifetime (s)	5×10^{-8}	$1 \cdot 6 \times 10^{-5}$	10^{-5}
$N_a - N_d$ the concentration of uncompensated acceptors (cm^{-3})	2.44×10^{12}	7.56×10^{13}	0.19×10^{10}
Diode quality factor	1.6	1.9	1.4
Series resistance (Ω. Cm^2)	1.08	2.5	2.1
Shunt resistance (Ω. Cm^2)	103	320	204

4. RESULTS AND ANALYSIS

Quantum dot size can be employed in all solar cells to reduce cost by saving usage materials size, enhance absorption and efficiency by controlling the size of the quantum dot size, since several properties can change due to any decrease in the size of the nanoparticles. This work discusses the benefit of reducing the quantum dot radii absorber and window layer radii on the performance of the heterojunction quantum dot thin film solar cells (ITO/QDCdS/QDPbS/Au), (ZnO/QDCdS/QDCIGS/Mo), (SnO₂/QDCdS/QDCdTe/Cu) models.

4.1. Optical characterization of quantum dot layers

Figure 1 shows radii effect on the refractive index and dielectric constant of quantum dot semiconductors CdS, CdTe, CIGS and PbS at wave length 500nm. It has been depicted that the refractive index and absolute dielectric constant of quantum dot (CdS, PbS, CIGS and CdTe) semiconductors have been lower than the refractive index and dielectric constant of bulk materials; because of decreasing the semiconductor material size. On the other hand, Figure 2 describes the effect of nanoparticles radii of quantum dot semiconductors layers (CdTe, CdS, PbS and CIGS) on the absorption coefficient and energy band gap at wave length 500nm and thickness 700nm.

4.2. New heterojunction quantum dot thin film solar cells

Figure 3 illustrates the short circuit current density, open circuit voltage, fill factor and efficiency of heterojunction quantum dot SnO₂/QDCdS/QDCdTe/Cu thin film solar cell with variant quantum dots CdS and CdTe radii. Whatever, Figure 4 describes the short circuit current density, open circuit voltage, fill factor and efficiency of heterojunction quantum dot Zno/QDCdS/QDCIGS/Mo thin film solar cell with variant of quantum dots CdS and CIGS radii. Figure 5 describes the short circuit current density, open circuit voltage, fill factor and efficiency of heterojunction quantum dot ITO/QDCdS/QDPbS/Au thin film solar cell with variant radii of quantum dot CdS and PbS. The traditional performance of heterojunction CdS/QDPbS has been enhanced by replacing the CdS and QDPbS layer with quantum dot QDCdS and QDPbS layers at radii 1nm or 1.35nm. It is noticed that. the best nanoparticles radii for window and absorber layers is 1nm for enhancing the open circuit voltage, short circuit current density, fill factor and energy conversion efficiency of the cell.

4.3. Comparison between traditional and heterojunction quantum dots solar cells

Figure 6 illustrated the benefit of using quantum dot size of window layer CdS instead of bulk one enhanced the absorption of window layer which result more enhancement in J-V and P-V characteristics. The enhancement in the J-V and P-V characteristics of traditional practical model has been occurred by using window layer CdS and absorber layer CdTe in quantum dot size with radii 1nm as shown in Figure 7. On the other hand, Figure 8 shows J-V and P-V characteristics of practical ZnO/CdS/CIGS/Mo model and proposal heterojunction quantum dot ZnO/QDCdS/QDCIGS/Mo thin film solar cell. Table 4 depicts the comparison in the performance of practical previous models [2, 3, 6] and the heterojunction quantum dot proposal models at room temperature. The table show that the performance of selected models has been enhanced by using window layer and absorber layer in quantum dot size with radii 1nm.
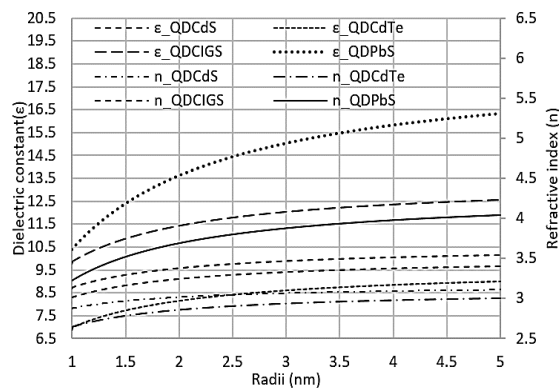

Figure 1. Radii effect on the refractive index and dielectric constant of quantum dot semiconductors CdS, CdTe, CIGS and PbS
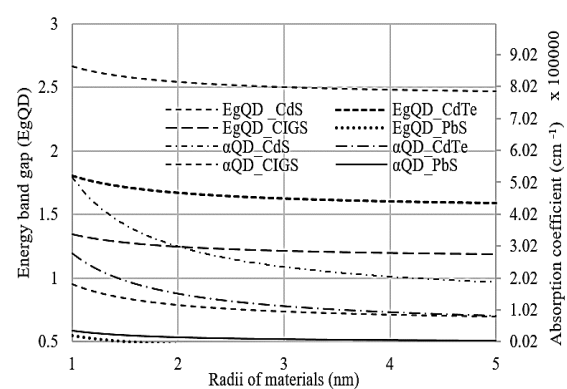
Figure 2. Radii effect on the absorption coefficient and energy band gap for quantum dot CdTe, CdS, PbS and CIGS layers at thickness 700nm
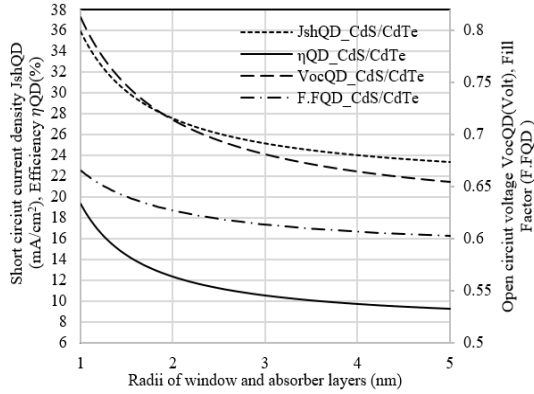
Figure 3. Quantum dots CdS and CdTe radii effect on the performance of heterojunction quantum dot SnO₂/QDCdS/QDCdTe/Cu thin film solar cell
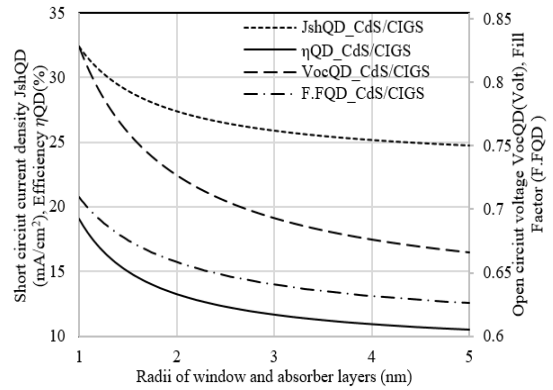
Figure 4. Quantum dots CdS and CIGS radii effect on the performance of heterojunction quantum dot ZnO/QDCdS/QDCIGS/Mo thin film solar cell
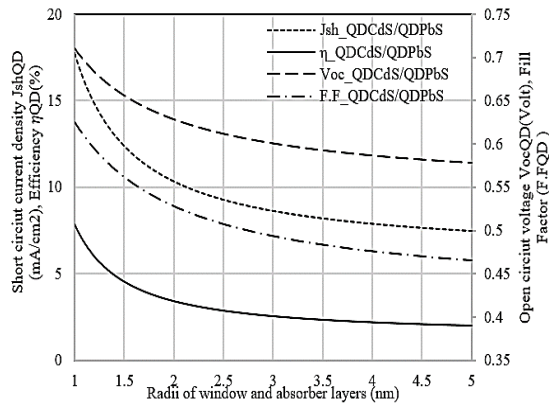
Figure 5. Quantum dots CdS and PbS radii effect on the performance of heterojunction quantum dot ITO/QDCdS/QDPbS/Au thin film solar cell
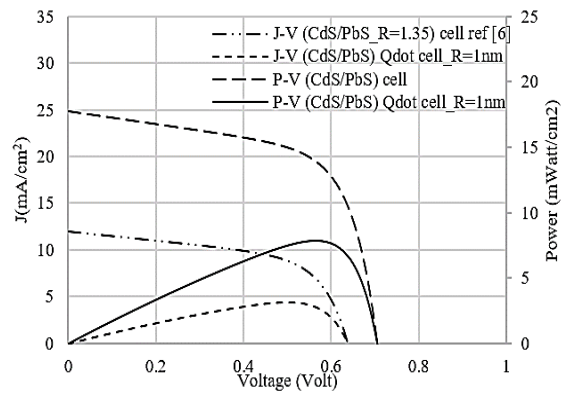
Figure 6. J-V and P-V characteristics of practical heterojunction quantum dot absorber layer CdS/QDPbS model and proposal quantum dot QDCdS/QDPbS thin film solar cell
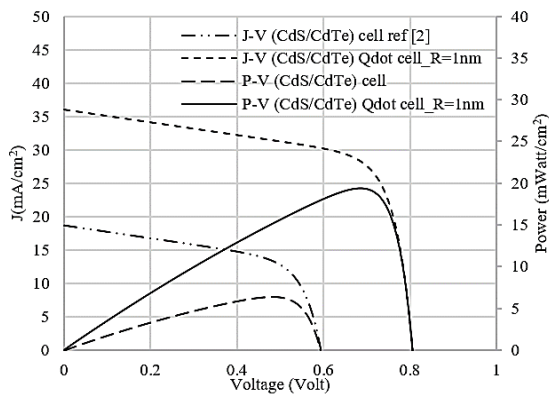
Figure 7. J-V and P-V characteristics of practical sub micro SnO₂/CdS/CdTe/Cu model and proposal heterojunction quantum dot SnO₂/QDCdS/QDCdTe/Cu thin film solar cell
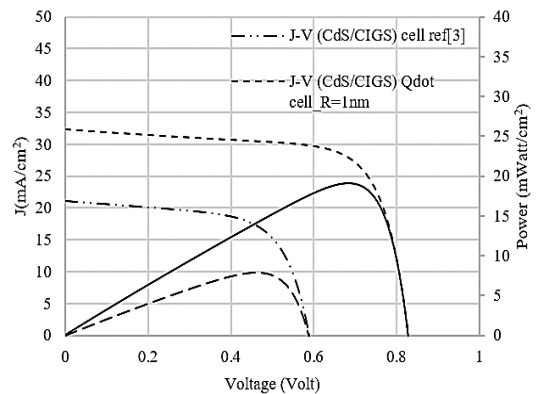
Figure 8. J-V and P-V characteristics of practical sub micro ZnO/CdS/CIGS/Mo model and proposal heterojunction quantum dot ZnO/QDCdS/QDCIGS/Mo thin film solar cell

Table 4. Comparison between efficiency and electric properties of traditional models and heterojunction quantum dot proposal models at room temperature

Cells	Open Circuit Voltage V_{oc} (Volt)	Short Circuit Current Density J_{sh} (mA/cm^2)	Fill Factor F.F	Efficiency (%)
CdS/ (QDPbS_R=1.35nm) [3]	0.63	12	0.43	3.3
(QDCdS/QDPbS)_R=1nm	0.71	17.75	0.63	7.88
(CdS/CdTe) [4]	0.58	18.6	0.65	4.7
(QDCdS/QDCdTe)_R=1nm	0.81	35.91	0.67	19.36
(CdS/CIGS) [5]	0.59	21	0.685	8.1
(QDCdS/QDCIGS)_R=1nm	0.83	32.43	0.71	19.05

5.   THERMAL EFFICIENCY ANALYSIS

Table 5 depicts the thermal effect on efficiency of proposal heterojunction quantum dot SnO2/QDCdS/QDCdTe/Cu, ZnO/QDCdS/QDCIGS/Mo, ITO/QDCdS/QDPbS/Au thin film solar cells at various radii of window and absorber layer materials CdS, CdTe. The energy conversion efficiencies of heterojunction quantum dots proposal thin film solar cells have been higher than the efficiency of practical models ZnO/CdS/CIGS/Mo, ITO/CdS/QDPbS/Au, SnO2/CdS/CdTe/Cu thin film solar cells under high thermal conditions.

Table 5. Comparison between proposal selected HJQD thin film solar cells and traditional practical previous models

Solar Cells	Efficiency %				
	300K	330 K	350 K	370 K	400 K
ITO/CdS/QDPbS/Au	1.47	1.25	1.11	0.98	0.82
SnO$_2$/CdS/CdTe/Cu	6.15	5.26	4.69	4.13	3.32
ZnO/CdS/CIGS/Mo	8.005	6.61	5.74	4.90	3.71
	Efficiency at radii 1nm				
ITO/QDCdS/QDPbS/Au	7.88	6.33	5.43	4.63	3.62
SnO$_2$/QDCdS/QDCdTe/Cu	19.36	17.34	16.03	14.75	12.88
ZnO/QDCdS/QDCIGS/Mo	19.05	16.40	14.81	13.31	11.17
	Efficiency at radii 1.5nm				
ITO/QDCdS/QDPbS/Au	4.57	3.72	3.22	2.78	2.5
SnO$_2$/QDCdS/QDCdTe/Cu	14.38	12.82	11.79	10.78	9.29
ZnO/QDCdS/QDCIGS/Mo	15.08	12.89	11.52	10.22	8.40
	Efficiency at radii 2nm				
ITO/QDCdS/QDPbS/Au	3.43	2.82	2.45	2.13	1.71
SnO$_2$/QDCdS/QDCdTe/Cu	12.32	10.94	10.03	9.14	7.83
ZnO/QDCdS/QDCIGS/Mo	13.36	11.34	10.08	8.89	7.19
	Efficiency at radii 3nm				
ITO/QDCdS/QDPbS/Au	2.56	2.12	1.86	1.63	1.32
SnO$_2$/QDCdS/QDCdTe/Cu	10.50	9.29	8.49	7.71	6.6
ZnO/QDCdS/QDCIGS/Mo	11.79	9.93	8.78	7.68	6.11

6.   CONCLUSION

The decrease in the grain size of CdTe, CIGS, CdS, PbS semiconductors to quantum dot size decreased the dielectric constant and refractive index. Whatever, using quantum dot size of CdTe, CIGS, CdS, PbS semiconductors increased the absorption coefficient of layers and energy band gap. Window and absorber layers' materials in quantum size enhanced the energy conversion efficiency, fill factor, short circuit current density, open circuit voltage of SnO$_2$/CdS/CdTe/Cu, ITO/CdS/QDPbS/Au and ZnO/CdS/CIGS/Mo thin film solar cells traditional models that are having sub-micro absorber layers' thicknesses and low efficiencies. Moreover, the reduction in radii of window and absorber layers materials in quantum dot size to be 1nm is the best radius for enhancing the performance of heterojunction quantum dot ITO/QDCdS/QDPbS/Au, ZnO/QDCdS/QDCIGS/Mo and SnO$_2$/QDCdS/QDCdTe/Cu cells due to increasing the energy band gap of absorber layer and increasing absorption of window and absorber layers which lead to decreasing the recombination and increasing the open circuit voltage, short circuit current density, output power density. Decreasing the size of quantum dot window and absorber layers' materials enhanced the performance of HJQD proposal selected cells at high temperatures.

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