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Ultra-optical characterization of thin film solar cells materials using core/shell absorber layer

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ABSTRACT

This paper investigates on new design of heterojunction quantum dot (HJQD) photovoltaics solar cells CdS/PbS that is based on quantum dot metallics PbS core/shell absorber layer and quantum dot window layer. It has been enhanced the performance of traditional HJQD thin film solar cells model based on quantum dot absorber layer and bulk window layer. The new design has been used sub-micro absorber layer thickness to achieve high efficiency with material reduction, low cost, and time. Metallics-semiconductor core/shell absorber layer has been succeeded for improving the optical characteristics such energy band gap and the absorption of absorber layer materials, also enhancing the performance of HJQD ITO/CdS/QDPbS/Au, sub micro thin film solar cells. Finally, it has been formulating the quantum dot (QD) metallic cores concentration effect on the absorption, energy band gap and electron-hole generation rate in absorber layers, external quantum efficiency, energy conversion efficiency, fill factor of the innovative design of HJQD cells.

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1. INTRODUCTION

Researchers are making considerable efforts to develop solar cells based on alternative materials because silicon is an indirect band gap material with a low absorption coefficient. Due to the low absorption, polycrystalline silicon solar cell structures must have a thickness in the range of 200 m, which makes the overall cost higher. We have earlier reported several non-silicon intermediate band gap materials that can be used for solar cell applications [1]–[4]. To overcome such limitations, thin-film solar cells, aiming at reducing cost by decreasing material consumption, will play an important role in future photovoltaic market. Unfortunately, a primarily unavoidable drawback of a thin-film solar cell is its poor optical absorption, which is caused by the thinner active layer and limits the power conversion efficiency with increasing temperature of this type of solar cells. To increase the optical absorption, different light trapping technologies have been extensively used to enhance the light absorption ability of thin-film solar cells [4]–[9]. The quantum dots (QDs) have been reported as promising third generation solar cells; quantum dots can be used in all Solar cells to decrease cost, increase absorption and efficiency by controlling the size of the quantum dots, since several properties can change due to any decrease in the size of nanoparticles [10], [11]. QDs have been incorporated different types of Solar cells such as: schottky solar cells, depleted heterojunction solar cells (SCs), hybrid organic/inorganic solar cells and quantum dot sensitized SCs [12]–[16]. The 3rd generation

technology nanostructured light trapping is a promising way to improve the efficiency in thin-film solar cells recently but it still under research due to their low efficiency [12]–[16]. Metal-semiconductor core/shell nanostructures have attracted a lot of attention due to their potential applications in optoelectronic devices. The metallic core enhances charge separation and improves absorption of light in the semiconductor during photo stimulation, so increasing the light harvesting efficiency of the semiconductor. When the differences in work function of the metal and semiconductor components and tune core/shell nanostructures during synthesis were tailored such as shell thickness and configuration of core and shell, the improved performance may be recognized. In addition, the interfacial structure may affect on the electronic properties of core−shell nanoparticles [17], [18]. The charge transfer in metal-semiconductor nanocomposites mechanism is used to approve a large improvement about 40 times of Au CdS core-shell, Also, the surface plasmon wave on gold surface can be used to excite electrons of Au to an excited state and transfer to the conduction band of CdS and recombine with holes in the valence band. So, it leads to the improved band gap and defect emissions in CdS nanostructures [19]. In this paper, the proposal model has been used the merits of QD metallic-semiconductor core/shell structure to enhance the performance of traditional CdS/QDPbS HJ-QDSc model. It has been used metallic- semiconductor core/shell absorber layer with quantum dot window layer to get high efficiency with lesser usage material based on sub micrometer thickness absorber layers [20]–[23].

2. DESIGN MODEL

Metal-semiconductor hetero-nanostructures exhibit different properties than the individual ingredients due to the intense interaction between metal and semiconductor. Surface plasmon resonances (SPR) in metal can be modulated by the semiconductor ingredient in hetero-structures. Through near-field interactions, energy could flow from the excited state of semiconductor to the plasmon, on the other side, plasmon-exciton interaction can also bring a modification of the radiative and nonradiative properties for semiconductor, changing the emission behaviors of semiconductor (enhancement or quenching). With appropriate band structures, charge transfer process like photo-excited electrons in semiconductor transferring to metal could suppress the direct recombination of carriers and promote efficient charge separation, resulting in a significant enhancement in the photoelectric conversion efficiency in solar cell [24]–[26]. The core-shell quantum dot dielectric function has been obtained using the maxwell garnett (MG) expression for spherical inclusions in explicit form [27].

$$\varepsilon_{efic-s} = \varepsilon_{shell} \frac{(\varepsilon_{core1} + 2\varepsilon_{shell}) + 2\digamma_{core1}(\varepsilon_{core1} - \varepsilon_{shell})}{(\varepsilon_{core1} + 2\varepsilon_{shell}) - \digamma_{core1}(\varepsilon_{core1} - \varepsilon_{shell})} \quad (1)$$

Where $\digamma_{core1}$ the core filling factor:

$$\digamma_{core1} = \left(\frac{R_1}{R_2}\right)^3 \quad (2)$$

R_1 radius of the quantum dot metallic core material. R_2 radius of the quantum dot semiconductor shell material. ε_{shell} is dielectric constant of quantum dot shell semiconductor layer material that described by drude model as shown in [28]–[31] as in (3):

$$\varepsilon_{shell} = \varepsilon_{shell\infty}\left(1 - \frac{\omega_b^2}{\omega^2 + i\omega(\gamma_{aQD})}\right) \quad (3)$$

where ω_b is the plasma angular frequency of semiconductor layer material and γ_{aQD} is the macroscopic damping constant.

To reflect the finite size of the nanoparticles, a term that depends on the size of the particle added to the damping constant as shown in (4).

$$y_{aQD} = \gamma_{mb} + \left(\frac{3v_{fb}}{4R}\right) \quad (4)$$

v_{fb} is the fermi velocity of semiconductor layer material. $\varepsilon_{shell\infty QD}$ is the infinity dielectric constant of QD semiconductor shell layer material which calculated as in (5).

$$\varepsilon_{shell\infty QD} = \varepsilon_o \left(1 + \frac{{\omega_b}^2}{\left(E_{g(Qdots)}\right)^2}\right) \quad (5)$$

$\varepsilon_{shell\infty QD}$ is the infinity dielectric constant of QD shell layer material which is lesser than the value of bulk material due to a lot of reasons; first, its nano-confined dimension that is lower than the incident wavelength so the refractive index reduces. Second reason, the refractive index of a semiconductor decreases with the increase in the energy band gap according to various empirical rules.

As shown in (5) the increase in the energy band gap of quantum dot material than the value of bulk material decreases the infinity dielectric constant. The refractive index in quantum dot thin films reduced so it is a great advantage in solar cells application where the reflection also decreased so absorption increases [31]–[34]. The energy band gap $E_{g(Qdots)}$ of quantum dot layer material can be approximated by [30]–[32].

$$E_{g(Qdots)} = E_{gbulk} + \frac{\pi^2 h^2}{2R^2}\left(\frac{1}{m_{eb}} + \frac{1}{m_{hb}}\right) - \frac{1 \cdot 8Q^2}{4\pi\varepsilon_b\varepsilon_o R_2} \quad (6)$$

Where

R_2 : radius of QD layer material
m_{eb} : the electron effective mass for layer material
m_{hb} : the hole effective mass for layer material
h : plank constant
ε_o : the permittivity of free space
Q : elementary charge

Varshni relation describe the temperature dependence of the bandgap in semiconductors which using in absorber or window layer as in [33]. ε_{core1} is dielectric constant of core metallic material that can be described by the drude model [35] as in (7):

$$\varepsilon_{core1} = \varepsilon_{INTRi} + 1 - \frac{\omega_{pi}^2}{\omega^2 + i\omega\left(\gamma_{mi} + \left(\frac{3v_{fi}}{4R_1}\right)\right)} \quad (7)$$

where, γ_{mi} is the macroscopic damping constant of core metallic material. ω_{pi}, v_{fi} are plasma angular frequency and fermi velocity of core metallic material.

The electron-hole generation rate in the core/shell absorber layer using individual metallic nanoparticles can be written based on [34], [35] as (8):

$$G_{ics}(\lambda) = \frac{\alpha_{bics}(\lambda)e^{-\alpha_{wiQD}(d_w)}[1 - R(\lambda)]\lambda I_o(\lambda)}{hc} \quad (8)$$

where, λ is wavelength, $I_o(\lambda)$ is the intensity of the solar spectral, c is the speed of light, h is Plank constant, $\alpha_{bics}(\lambda)$ is the absorption of the core-shell absorber layer. α_{wiQD} is the absorption of quantum dot window layer in core-shell thin film solar cells. $\alpha_{bics}(\lambda)\ and\ \alpha_{wiQD}$ can be calculated by the Beer-Lambert's law based on refractive index of layers as [31], [35].

Whatever, $J_{diodics}(V)$ is the forward diode current for heterojunction quantum dot thin film solar cell based on core/shell absorber layer and quantum dot window layer based on [33]–[35] as in (9):

$$J_{diodics}(V) = J_{Oics}\left(exp\left(\frac{Q(V + J(V)R_{ser})}{nKT}\right) - 1\right) \quad (9)$$

J_{Oics} is reverse saturation current density in new design for heterojunction quantum dot thin film solar cells based on metallic-semiconductor core/shell absorber layer calculated based on ref. [31], [35]. Where, V is applied voltage. J_{Oics} is reverse saturation current density in HJQD cells using metallic-semiconductor core/shell absorber layer. R_{ser} is the series resistance. n is diode ideality factor. T is absolute temperature.

E_{gbics} is the energy band gap of core/shell absorber layer material that is affected by the metallic nanoparticles. The energy band gap of a semiconductor enhances with decreasing refractive index according to various empirical rules and expressions of refractive index and energy band gap. The energy band gap of metallic-semiconductor core/shell absorber layer material E_{gbi} calculated as shown [35], [36]:

$$E_{gbics} = \frac{36.3}{e^{n_{fic-s}}} \tag{10}$$

The total photo generated current density $J_{phics}(V)$ using quantum dot metallic-semiconductor core/shell absorber layer and quantum dot window layer which obtained by integrating over all incident photon wavelengths of the solar spectrum [31], [34], [35].

$$J_{phics}(V) = \int_0^{\infty} J_{Tics}(\lambda.V)d\lambda \tag{13}$$

Where, the resultant photocurrent density $J_{Tics}(\lambda.V)$ and the net external current density $J_{indcs}(V)$ from a solar cell that is quantum dot metallic-semiconductor core/shell absorber layer and quantum dot window layer and the open circuit voltage equation is expressed as in [31], [34], [35].

$$J_{indcs}(V) = J_{phics}(V) - J_{dics}(V) - \left(\frac{V + J(V)R_{ser}}{R_{sh}}\right) \tag{14}$$

Where, R_{sh} is the shunt resistance:

$$V_{ocics} = \left(\frac{KT}{Q}\right)\ln\left[\frac{J_{phics}}{J_O} + 1\right] \tag{15}$$

The output power density of the new heterojunction quantum dot solar cell based on metallic-semiconductor core/shell absorber layer structure and QD window layer.

$$P_{ics} = J_{phics} \times V \tag{16}$$

P_{maxics} is the maximum power point density of the proposals cells which estimated from P_{ics} −V curve.

On the other hand, the calculation of fill factor to an excellent accuracy and the final equation for the efficiency of the new heterojunction quantum dot solar cell based on metallic-semiconductor core/shell absorber layer structure and quantum dot window layer as in [35] as in (17):

$$F.F_{icore-shell} = \frac{P_{maxics}}{V_{ocics} \times J_{phics}}$$
$$\eta_{icore-shell} = \frac{J_{phics}V_{ocics}F.F_{icore-shell}}{P_{in}} \times 100 \tag{17}$$

Whatever, the external quantum efficiency $EQE_{icore-shell}(\lambda)$ of the new heterojunction quantum dot solar cell based on metallic-semiconductor core/shell absorber layer and quantum dot window layer structure has been calculated by (18) [35]:

$$EQE_{icore-shell}(\lambda) = \frac{J_{phics}(\lambda)}{Q\emptyset(\lambda)} \tag{18}$$

where, $\emptyset(\lambda)$ is the spectral photon density.

3. SELECTED MATERIALS AND PARAMETERS OF MODELS

The aim of this paper is improving the efficiency and performance of traditional models that are based on sub micro absorber layer thickness for achieving high efficiency with less absorber layer thickness for reductional cost of materials by using metallic-semiconductor core/shell absorber layer of selected HJQD models. Thus, the core/shell absorber layer thin film solar cells materials parameters are achieved high efficiency and J-V characteristics of ITO/CdS/PbS/Al with respect to traditional HJQD models [21], [31].

Table 1 and Table 2 show the main parameters of usage materials and parameters of HJQD thin film models based on QD window layer and metallic-semiconductor core/shell absorber layer; the results have been obtained using QD window layer radius 1 nm and QD core/shell with QD shell layer material radius 3nm and under AM1.5 solar irradiation.

Table 1. Parameters of proposal HJQD cells models based on core/shell absorber layer and QD window layer [21], [31]

Parameters	CdS/PbS
Absorber layer thickness (nm)	500
Window layer thickness (nm)	100
Front layer thickness (nm)	100
Electron lifetime (s)	10^{-9}
Hole lifetime (s)	10^{-9}
$N_a - N_d$ the concentration of uncompensated acceptors (cm^{-3})	0.19×10^{10}
Diode quality factor	1.4
Series resistance (Ω. Cm^2)	2.1
Shunt resistance (Ω. Cm^2)	204

Table 2. Characteristics of usage materials as substrate layer or QD core materials in QD shell absorber layer for HJQD thin film models [35]

Materials	Plasma angular frequency ($\omega_p 10^{16}$rad/s)	Damping constant (γ_m 10^{13} s^{-1})	Fermi velocity (v_f 10^6m/s)
Cesium (Cs)	0.54	0.756	0.75
Lithium (Li)	1.225	1.85	1.29
Cupper (Cu)	1.03	5.26	1.57
Silver (Ag)	1.40	2.80	1.39
Aluminum (Al)	1.09	12.4	2.03
Molybdenum (Mo)	0.19	1.13	-

4. RESULTS AND DISCUSSION

The behavior and characterization of the innovative design of heterojunction quantum dot of photovoltaic solar cell which based on QD window layer and QD core-shell absorber layer has been layout as follows: Figure 1 shows the metallic cores concentration effect on the optical characteristics of metallic-PbS core/shell absorber layers for new HJQD (QDCdS/QDPbS). Figure 1 shows that using metallic-PbS core/shell structure enhanced the optical characteristics of QDPbS with increasing the concentration of metallic cores (Ag, Cu, Li or Al) inside QDPbS shell by decreasing dielectric constant, refractive index, increasing energy band gap so the absorption coefficient and electron -hole generation rate in QDPbS layer enhanced. Figure 2 shows the quantum dot metallic cores concentration effect on the generation rate and absorption coefficient in absorber layer of heterojunction quantum dot CdS/PbS thin film solar cell. Using Silver, Copper, Aluminum, Cesium or Lithium quantum dot cores in quantum dot PbS shell layer increased the electron-hole pair generation rate in the PbS absorber layer. The absorption coefficient of metallics-PbS core/shell absorber layer increased by increasing the volume fraction. Cesium has been the best quantum dot core for enhancing the absorption coefficient, then; quantum dot Copper core has been the second order for improving the absorption coefficient. Silver has been the least one for improving the absorption coefficient of PbS shell layer.

On the other hand, Figure 3 describes the joint venture (JV) and photovoltaic (PV) characteristics of heterojunction quantum dot ITO/CdS/PbS/Au thin film solar cells based on quantum dot core-shell absorber layer and quantum dot window layer. The short circuit current density, open circuit voltage and maximum output power density of heterojunction quantum dot CdS/PbS thin film solar cells has been increased by using 20 wt% of Silver, Aluminum, Lithium, Copper or Cesium quantum dot cores in the QD PbS shell layer due to increasing the optical properties of quantum dot PbS shell layer and declining the reverse saturation current density of the cell. The most enhancements have been occurred by using quantum dot Cesium core in the quantum dot PbS absorber layer with increasing the wavelength. Copper has been the second order for enhancing the external quantum efficiency of heterojunction quantum dot ITO/CdS/PbS/Al thin film solar cell.

Figure 4 shows the quantum dot metallic cores concentration effect on the energy conversion efficiency and fill factor of heterojunction quantum dot CdS/PbS thin film solar cell based on quantum dot window layer and quantum dot metallics-PbS core/shell layer material. Anew solar cell design that using quantum dot metallic cores of Silver, Copper, Lithium, Aluminum or Cesium in PbS quantum dot shell layer could raise the energy conversion efficiency and fill factor of heterojunction quantum dot CdS/PbS thin film solar cell with increasing the volume fraction. The external quantum efficiency of heterojunction quantum dot CdS/PbS thin film solar cells has been increased by using 20 wt% of Silver, Aluminum, Lithium, Copper or Cesium quantum dot cores in the QD PbS shell layer due to increasing the optical properties of quantum dot PbS shell layer and declining the reverse saturation current density of the cell.

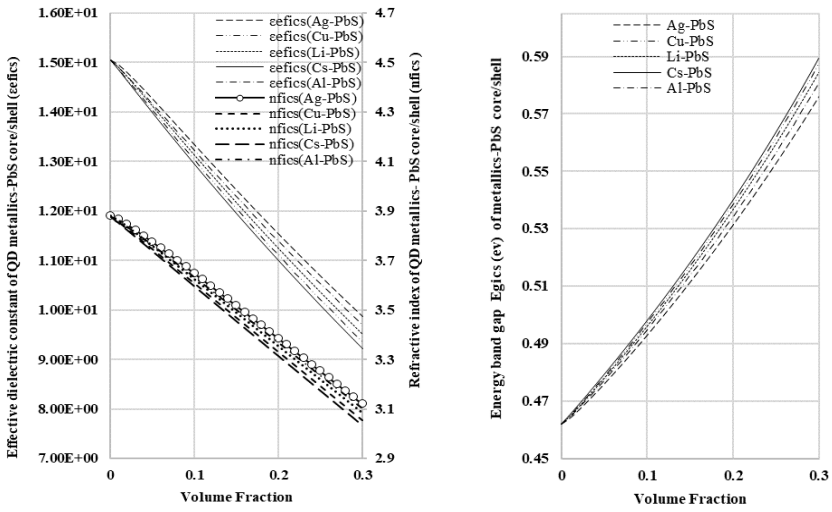

Figure 1. Refractive index, Effective dielectric constant and energy band gap of QD metallics-PbS core/shell

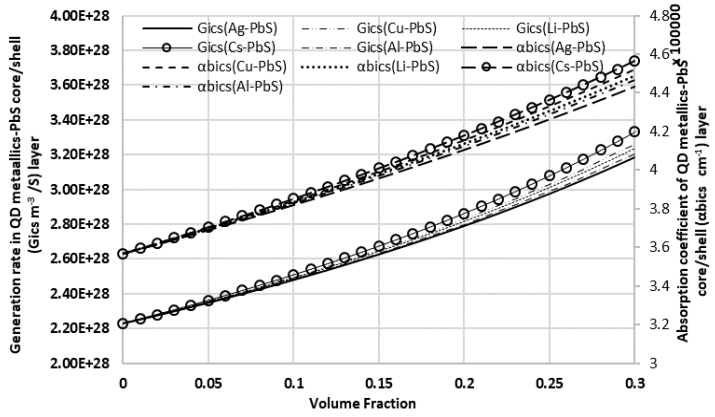

Figure 2. Generation rate, absorption coefficient and reverse saturation current density in PbS shell layer of heterojunction quantum dot ITO/QDCdS/metallics-PbS/Au thin film solar cell

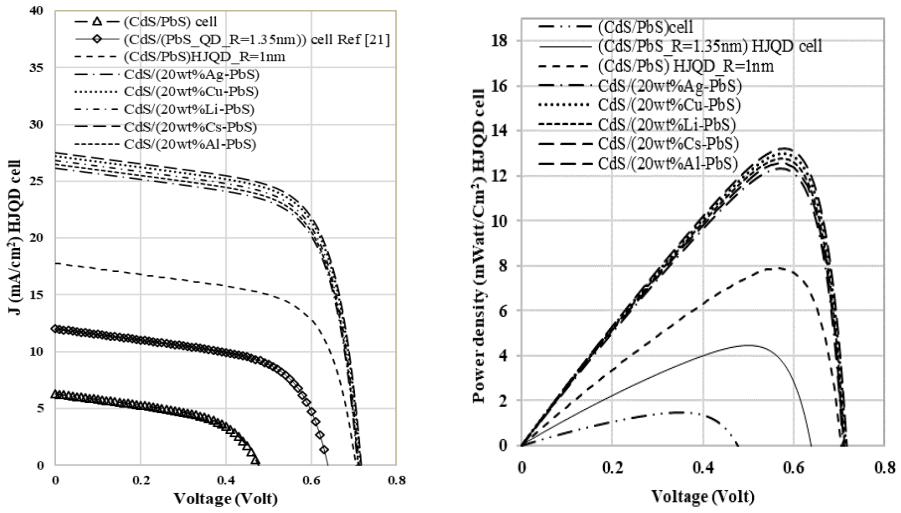

Figure 3. J-V and P-V characteristics of heterojunction quantum dot ITO/QDCdS/metallics-PbS/Au thin film solar cells

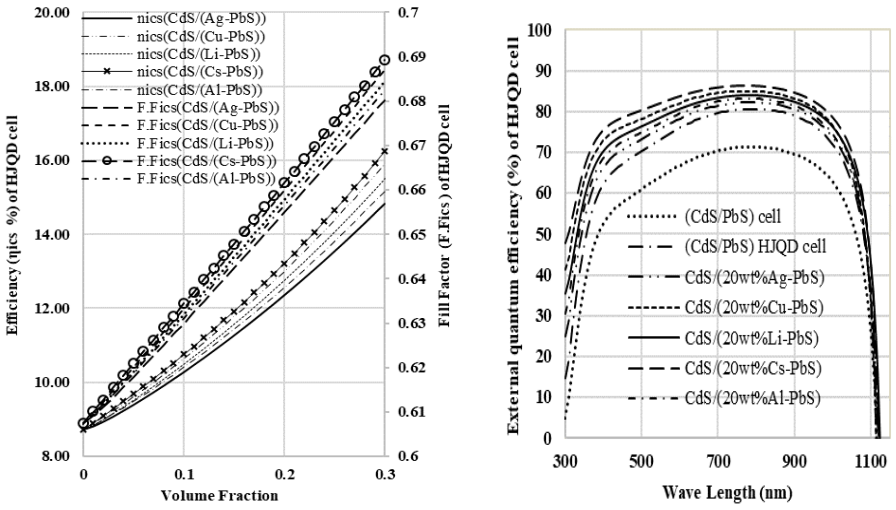

Figure 4. Fill factor, energy conversion efficiency and external quantum efficiency of heterojunction quantum dot ITO/QDCdS/metallics-PbS/Au thin film solar cell

5. CONCLUSION

Quantum dot aluminum, lithium, cesium, copper or silver core concern to reduce the dielectric constant and refractive index of PbS shells. On the other side, the energy band gap of PbS shell enhanced with increasing the volumetric concentration of selected metallics core. The absorption coefficient and electron hole generation rate of metallics-PbS core/shell absorber layer has been increased by increasing the volume fraction of the proposed metallics cores. The enhancement in the energy band gap and the electron-hole generation rate results increasing in the open circuit voltage, short circuit current, the maximum power point and so efficiency of HJQD CdS/PbS thin film. Cesium has been the best quantum dot core for enhancing the performance of HJQD CdS/PbS cell, then; QD Cu core has been the second order for improving the performance of HJQD CdS/PbS cell. However, QD Silver core has been the least one for improving the performance of HJQD CdS/PbS cell

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