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Course: Quantum Transport and Logic Gates

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Project On:

Analysis of Heterojunction Solar Cells with Quantum Dot Integration

Project By

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ABSTRACT

Heterojunction solar cells (HJT), variously known as Silicon heterojunctions (SHJ) or Heterojunction with Intrinsic Thin Layer (HIT),[1] are a family of photovoltaic cell technologies based on a heterojunction formed between semiconductors with dissimilar band gaps. They are a hybrid technology, combining aspects of conventional crystalline solar cells with thin-film solar cells. Heterojunction solar cells are composed of two different materials- two semiconductors or a semiconductor and an electrolyte. A photovoltaic cell combines two functions that permit conversion of photons flux to electric power. One, numerous semiconductors in a semiconductor when it is made into a diode. This space charge separates the photoexcited electron from the unoccupied ground state, the hole, coming photon as photovoltage.

INTRODUCTION

With endless energy demand and climate change issue, solar cells [1] which convert sunlight directly into electricity are becoming increasingly important in the world's renewable energy mix. The development of news solar cell technologies with lower production costs is therefore of great interest to industry. New and prospective materials are under intensive research in order to create low cost and highly efficient photovoltaic devices based on various organic,hybrid organic inorganic, and inorganic heterojunctions. Heterojunction solar cells possess a combination of unique properties of different materials that help to improve their operational characteristics compared with traditional homo junction silicon solar cells.

The operation of these solar cells relies on the interaction of incoming photons with the semiconductor material, which leads to the generation of electron-hole pairs. These carriers are then separated by the internal electric field of the junction, generating a photovoltage. To further improve the efficiency and spectral response, the incorporation of quantum dots (QDs) — semiconductor nanocrystals with discrete energy levels — has been proposed. QDs can act as intermediate band absorbers, enabling enhanced photon absorption and carrier generation.

Heterojunction solar cells are investigated not merely because they offer another method of diode formation. To list a simple classification, heterojunctions are required for or are the result of: a) surface passivation and high sheet conductance; b) monolithic multi junction cells; c) semiconductors that exhibit only one conductivity type ; d) fabrication at low temperatures.

It is here that we first replicate the conventional energy band diagram of an HJT cell to have a reference point. Next, we alter the diagram to incorporate quantum dots in an appropriate layer and explore their effects on device performance. The research identifies how quantum dots impact carrier transport, recombination, and solar cell performance, and presents information on their operating response in future photovoltaic architectures.

OBJECTIVE

To demonstrate the energy band diagram and carrier dynamics of a Heterojunction Solar Cell, supported by relevant cross-referenced studies. Further, to investigate the impact of incorporating Quantum Dots into a suitable layer of the cell by modifying and reproducing the same figure for this enhanced configuration. The objective also includes analysing and highlighting the role and response of Quantum Dots during the solar cell's operation, particularly in terms of performance enhancement and carrier transport.

DESIGN AND ANALYSIS

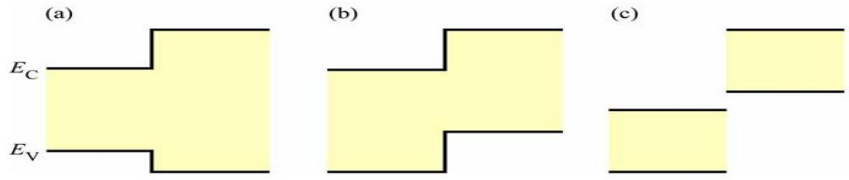


Fig.1.Types of energy band lineups: (a) type I-straddled (b)type II-staggered (c)type III-broken gap

We classify heterostructures [2] according to the alignment of the bands of the two semiconductors. Three different alignments of the conduction and valence bands and of the forbidden gap are shown in *Fig.1*. *Fig.1(a)* shows the most common alignment which will be referred to as the straddled alignment or "Type I" alignment. The most widely studied heterostructure, that is the GaAs / $Al_xGa_{1-x}As$ heterostructure, exhibits this straddled band alignment.*Fig.1(b)* shows the staggered lineup. In this alignment, the steps in the valence and conduction band go in the same direction. The staggered band alignment occurs for a wide composition range in the $Ga_xIn_{1-x}As$ / $GaAs_ySb_{1-y}$ material system. The most extreme band alignment is the broken gap alignment shown in *Fig.1(c)*. This alignment occurs in the InAs / GaSb material system. Both the staggered lineup and the broken-gap alignment are called "Type II" energy band alignments. At the semiconductor interface of the heterostructure, the energies of the conduction and valence band edges change. The magnitudes of the changes in the band-edge energies are critically important for many semiconductor devices.Among the many solar cells available, perovskite solar cells (PSCs) stand out for their excellent photovoltaic properties. PSCs usually consist of the electron transport layer (ETL), the light-absorbing layer and the hole transport layer (HTL). The ETL is generally TiO2, SnO2, phenyl-C61-butyric acid methyl ester (PCBM).

Mathematical Theory Approach

Basic semiconductor equations had to be solved in order to assess the performance of the solar cell; these equations have a real-valued function. The following equations[3], which explain the physical models utilized for this simulation, can be used to describe solar cell operation: The Poisson equation, which connects charge to electrostatic potential, is the governing equation. Equation (1) contains the Poisson Electrostatic Potential equation.

$\frac{d^2E}{dx^2} = \rho/E$...(1), where rho being the charge density (C.cm-3), and epsilon is the substance permittivity. Equation (2), which is derived from the charge neutrality equation, can be written as the dopant fully ionized.

$\rho = q(p - n + N_D^+ - N_A^-)/\varepsilon$.... (2), The second equation is a continuity equation, which is also known as a governing equation because it considers generation, recombination, drift, and diffusion simultaneously. The continuity equation for the change in electron and hole concentration is represented by equations (4) and (5)

$\frac{\partial n}{\partial t} = G_n - R_n + \frac{1}{q}.\frac{\partial J_n}{\partial x}$ and $\frac{\partial p}{\partial t} = G_p - R_p + \frac{1}{q}.\frac{\partial J_p}{\partial x}$ ....(4),(5). Where the current density of the electrons is Jn, while the current density of the holes is Jp, Gn and Gp represent the rates of creation of electrons and holes, respectively, and Rn and Rp represent the rates of recombination of electrons and holes.

IMPLEMENTATION

Type 1 - Straddled

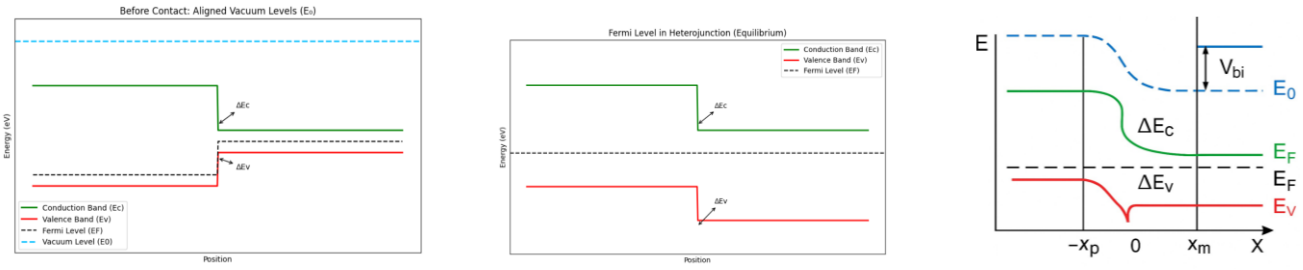
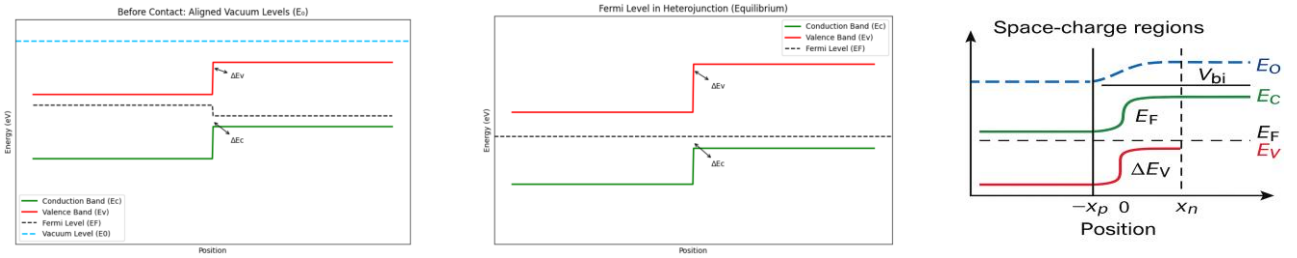


Fig.2.

Type 2 - Staggered



Type 3 -Broken gap

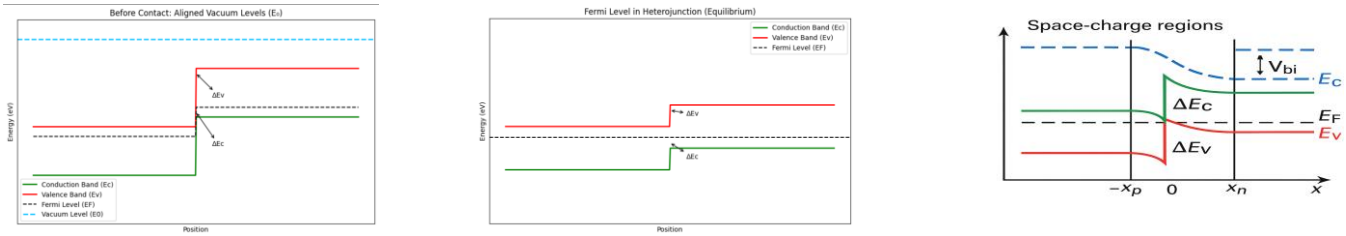


Fig.2(a),(b),(c) Schematic band diagrams for three typical heterojunctions with aligned vacuum level E0 (type I-straddled, type II-staggered, type III-broken gap), brought into thermodynamic equilibrium resulting in an aligned Fermi level, and brought into contact with compensating space-charge regions.

Quantum Dots as Additives in Electron Transport Layers

The electron transport layer (ETL) has the function[4] of collecting and transporting electrons to the conductive glass, while effectively blocking holes from recombination. The ideal electron transport material (ETM) should have the following properties:
(1) Proper alignment of energy levels to allow for the efficient extraction of electrons.
(2) High electron mobility to transfer the photogenerated electrons to the external circuits faster. However, electron transport and extraction in the ETL of PSCs are not ideal, showing stability and hysteresis issues. QDs doping into ETL presented an effective method for optimizing ETM.

INCLUDING QUANTUM DOTS

Carbon is a popular building material due to its low price, high surface area and abundant resources. Doping carbon materials into PSCs can significantly improve [5] the PCE and stability. Carbon quantum dots (CQDs) and graphene quantum dots (GQDs) are widely used in PSCs due to their excellent properties. CQDs are zero-dimensional carbon-based materials, with sizes less than 10 nm. CQDs consist of dispersed sphere-like carbon particles. It is mainly doped into ETL such as TiO2, SnO2 and PCBM to improve the performance of PSCs and increase PCE. TiO2 has the disadvantages of low electron mobility ($\sim 10^{-4}$ $cm^2 V^{-1} s^{-1}$) and low conductivity ($\sim 1.1 \times 10^{-5} Scm^{-1}$). Under UV light, it has strong photocatalytic effects that can easily cause the decomposition of perovskite. To solve the problem of slower charge transfer, we present usage of composites of treated CQDs with TiO2 as ETL for PSCs.

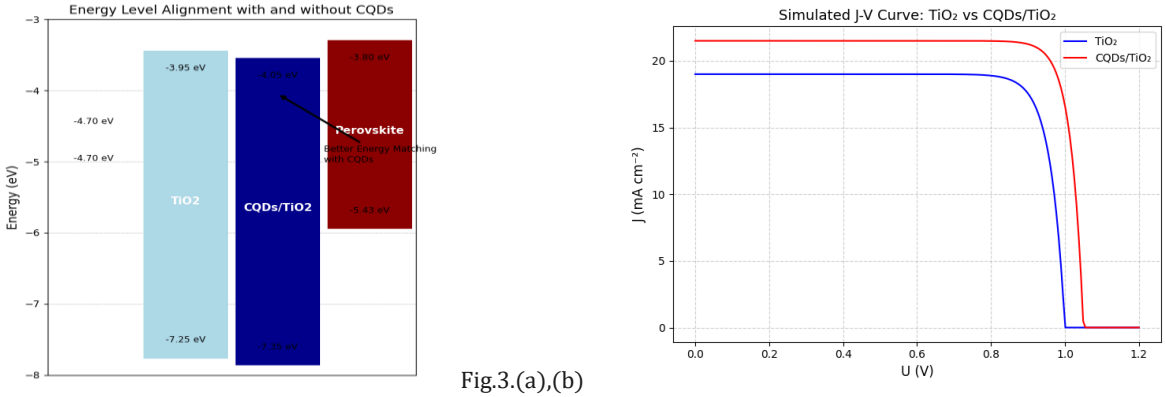


Fig.3.(a),(b)

Fig.3. (a)solving the problem of slower charge transfer by using composites of treated CQDs with TiO2 as ETL for PSCs showing that CQDs can enhance electron extraction and electron coupling between the perovskite and ETL. Fig.3.(b)TiO_2(blue): lower current and earlier roll-off, CQDs/TiO_2 (red): improved current density and voltage.It mimics the experimental performance boost due to enhanced electron extraction by CQDs.

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=== Performance Parameter: Efficiency (η) ===
Without CQDs: 14.82 %
With CQDs   : 17.61 %
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Fig.4.(a)

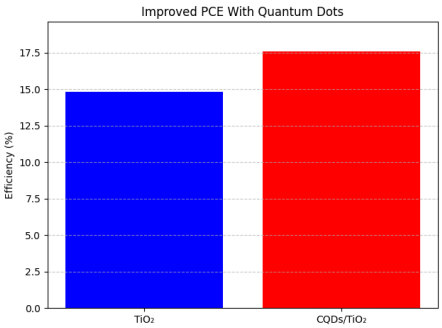
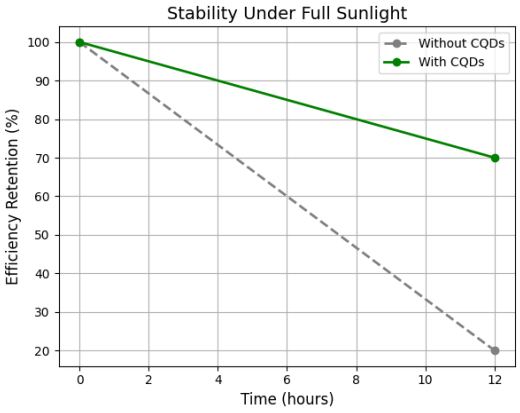
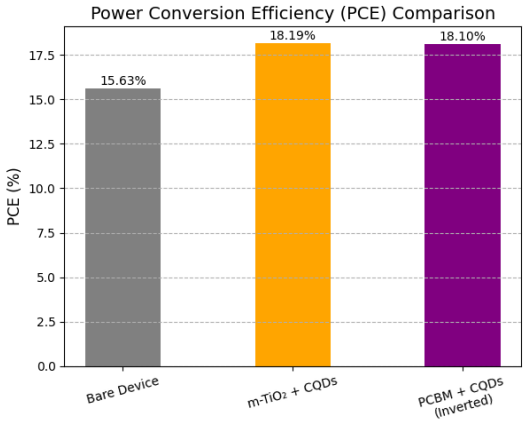


Fig.4.(b)

Fig.4.(a) Achieving better energy level matching and ultimately contributing to the high performance of the device, with a **PCE of 17.61%**.

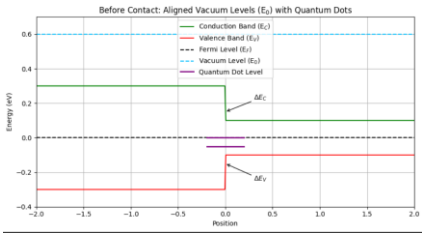
Fig.4.(b)Introduced CQDs in the mesoporous TiO2(m-TiO2) layer in PSCs using the modified hydrothermal method to prevent the UV-induced decomposition of perovskite films. CQDs effectively converted UV light into blue light and significantly enhanced the light stability of PSCs. In total, 70% of the initial efficiency was maintained after 12 h of full sunlight, much higher than the 20% initial efficiency of the bare device. Finally, the PCE had **improved to 17.61%**. The CQDs not only substantially increased the electron mobility, but also effectively prevented I- ions from undergoing interfacial diffusion and inhibited the decomposition of perovskite, resulting in enhanced long-term device stability and a **final PCE of 18.1% for the inverted PSCs.**

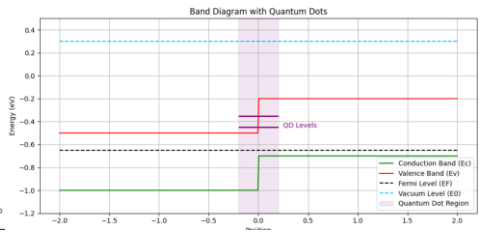




PCE	**EFFICIENCY (%)**
Bare device	15.63
m-TiO2+CQDs	18.19
PCMB+CQDs(inverted)	18.10

Including Qdots in heterojunction band diagrams





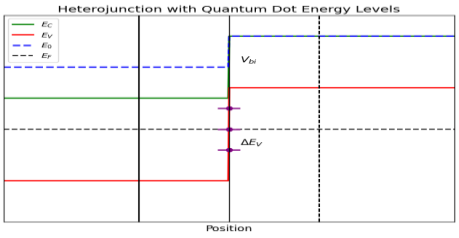


Fig.5.(a) Fig.5.(b) Fig.5.(c)

In Fig.5.(a), the band alignment before contact shows the integration of quantum dots (QDs) at the interface of two semiconductors. The QD levels, placed between the conduction and valence bands, create intermediate states that can facilitate carrier transition, enhancing charge separation and reducing recombination losses. The conduction band offset (ΔEc) and valence band offset (ΔEv) further illustrate the potential barriers carriers must overcome, with QDs acting as energy stepping stones.In Fig.5.(b), the QDs are embedded within the active region, forming discrete energy states (marked in purple) that lie within the bandgap. These localized states promote photon absorption and extend the spectral response of the material. This configuration can improve photocarrier generation, particularly in low-energy regions, and offer multiple carrier excitation pathways.In Fig.5.(c) shows a heterojunction modified by quantum dots, where the QD levels appear at the interface. The built-in potential (Vbi) is maintained while the QD levels offer intermediate energy states for charge carriers. This can enhance charge extraction efficiency by minimizing energy losses during transport across the junction, making the structure highly beneficial for photovoltaic or optoelectronic applications.

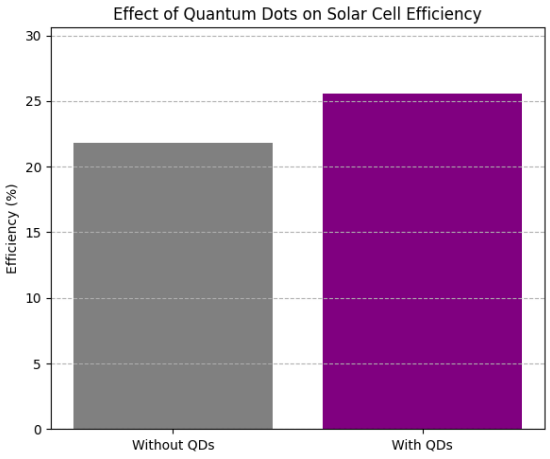


Fig.6.(a)

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=== Without Quantum Dots ===
Voc: 1.05 V, Jsc: 26 mA/cm², Efficiency: 21.84 %

=== With Quantum Dots ===
Voc: 1.0 V, Jsc: 32 mA/cm², Efficiency: 25.60 %
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Fig.6. (b)

Fig.6.(a) The integration of quantum dots enhances solar cell performance primarily by increasing the short-circuit current density (Jsc), which suggests improved light absorption or carrier collection due to intermediate QD energy levels. Fig.6.(b)Despite a minor drop in Voc, the **overall efficiency improves by ~3.8%**, highlighting the effectiveness of QDs in boosting photocurrent generation and extending spectral response.This supports the role of QDs in facilitating carrier transitions and improving device output, particularly in photovoltaic applications.

RESULTS & CONCLUSION

Parameter	TiO_2	CQDs/TiO_2	Inference
Short-Circuit Current	~26 mA/cm²	~32 mA/cm²	CQDs enhance light absorption and charge extraction, increasing current output.
Open-Circuit Voltage	~1.05 V	~1.00 V	Better energy level alignment improves charge separation and boosts V.
Curve Shape	Sharper drop-off	Smoother transition	Reduced recombination due to CQDs improves diode quality and efficiency.
Performance Trend	Lower	Higher	CQDs contribute to improved photovoltaic performance.

Material	Type	Role/Use in PSC	Properties
Carbon	Building Material	Base material for Qdots	Low cost, high surface area, abundant
CQDs	Qdot (Carbon)	Doped into ETL (TiO_2, SnO_2, PCBM)	<10 nm size, excellent electron transfer, broad light absorption, high mobility
TiO_2	ETL	Host for CQD doping	Standard ETL with good stability
SnO_2	ETL	Host for CQD doping	High electron mobility, better conduction
PXMB	ETL	Host for CQD doping	Common ETL in inverted architectures

The addition of quantum dots (QDs) to perovskite solar cells (PSCs) shows a significant enhancement in power conversion efficiency (PCE) in different device architectures. For example, whereas a pristine device has a PCE of 15.63%, adding carbon quantum dots (CQDs) to the mesoporous TiO_2 (m-TiO_2) layer increases efficiency to 18.19%, and CQD doping in the PCBM layer for inverted devices leads to a comparable enhancement to 18.10%. This ~3.8% gain owes mainly to a higher short-circuit current density (Jsc), caused by improved carrier collection and light harvesting due to the intermediate energy levels of the QDs. To support this, simulations indicate that Jsc rises from 26 mA/cm^2 to 32 mA/cm^2 with QD incorporation while the open-circuit voltage (Voc) drops slightly from 1.05 V to 1.00 V—showing that QDs mainly boost photocurrent without drastically impairing voltage. Overall, efficiency increases from 21.84% to 25.60%, highlighting the significant role of QDs in maximizing charge transport, enhancing spectral absorption, and ultimately improving the performance of PSCs.

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