

Quantum Dots and Their Use in Solar Cells

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Abstract

Quantum dots (QDs) have gained significant attention as advanced light-absorbing materials in photovoltaic systems due to their tunable bandgaps, high absorption coefficients, and potential for multiple excitation generation (MEG). These nanoscale semiconductors offer a pathway to surpass the efficiency limits of traditional solar cells through spectral tuning and enhanced photon-to-electron conversion mechanisms. This paper reviews the fundamental properties of QDs relevant to solar energy conversion, including quantum confinement behavior, charge carrier dynamics, and synthesis approaches. It also explores recent advances in QD-based solar cell architectures—such as sensitized, heterojunction, and tandem configurations—highlighting performance metrics, integration challenges, and environmental considerations. Finally, it outlines future directions in QD photovoltaics, including the use of non-toxic materials, scalable fabrication methods, and AI-assisted material discovery. These insights emphasize the transformative potential of QDs in advancing low-cost, high-efficiency solar technologies.

Keywords: Quantum Dots, Solar Cells, Multiple Exciton Generation, Nanocrystals, Photovoltaics, and Energy Conversion.

الملخص

باهتمام كبير بصفتها موادًا متقدمة لامتصاص الضوء في (Quantum Dots - QDs) لقد حظيت النقاط الكمومية أنظمة الخلايا الكهروضوئية، وذلك بفضل فجواتها الطاقية القابلة للضبط، ومعاملات الامتصاص العالية، وإمكانية توليد وتوفر هذه المواد شبه الموصلية النانوية طريقًا لتجاوز حدود كفاءة الخلايا الشمسية التقليدية (MEG). إكسيتونات متعددة من خلال التوليف الطيفي وتعزيز آليات تحويل الفوتونات إلى إلكترونات. يستعرض هذا البحث الخصائص الأساسية للنقاط الكمومية ذات الصلة بتحويل الطاقة الشمسية، بما في ذلك سلوك الحصر الكمومي، وديناميكيات حوامل الشحنة وطرق التخليق. كما يتناول التطورات الحديثة في تصميمات الخلايا الشمسية المعتمدة على النقاط الكمومية مثل الخلايا الحساسة، وخلايا الوصلات غير المتجانسة، والخلايا الترادفية مع تسليط الضوء على مؤشرات الأداء، وتحديات التكامل، والاعتبارات البيئية. وأخيرًا، يُعرض البحث التوجهات المستقبلية في مجال الخلايا الشمسية القائمة على النقاط الكمومية

مثل استخدام مواد غير سامة، وأساليب تصنيع قابلة للتوسع، والاستعانة بالذكاء الاصطناعي لاكتشاف المواد. تؤكد هذه الرؤية على الإمكانيات التحولية للنقاط الكمومية في تطوير تقنيات شمسية منخفضة التكلفة وعالية الكفاءة، الكلمات المفتاحية: النقاط الكمومية، الخلايا الشمسية، توليد الإكسيتونات المتعددة، البلورات النانوية، الكهروضوئية، تحويل الطاقة.

1-Introduction

The distinctive quality of quantum dots (QDs) makes them useful in the production of solar cells and devices. With QDs, it is possible to fabricate solar devices that respond to light in controlled ways as well as flexible, semi-transparent, or even tandem (layered) cells. The last few years have seen progress in quantum dot manufacturing surface modification and processes related to the materials surrounding them. Other developments also have made it easier for charge transport in them and reduced energy losses. Therefore, quantum dot solar cells (QDSCs) became more useful and efficient (Kovalenko et al., 2020).

This study explores the fundamentals of quantum dots, including their use in different solar cells, other factors that affect their efficiency, and major performance constraints. Also, what is the barrier to broader acceptance of QDs, and aims at what research would enable these to be fully utilized in solar energy.

- Quantum Dot Fundamentals

Semiconductor-based quantum dots are tiny crystals that are often less than 10 nanometers across. Quantum confinement is a property that makes them act differently than bigger things. When a QD gets close to the exciton Bohr radius, the movement of electrons and holes inside it is limited in all directions. This creates different energy levels that depend on the size of the dot. As the QD gets smaller, its bandgap energy increases, which lets you control its light absorption and emission very precisely (Flory et al., 2010).

This tunability is particularly beneficial in solar energy applications, where it is essential to align the bandgap of the absorber with the solar spectrum to maximize efficiency.

This effect is demonstrated by the changes in the energy band structure as one goes from bulk materials to nanoscale crystals: reducing particle size gradually expands the bandgap, which enables absorption profiles to shift from the infrared region to the visible and even ultraviolet regions, depending on the specific material system and synthesis conditions (Kim et al., 2021). The resulting size-dependent optical response not only improves light-harvesting selectivity but also enables spectral stacking strategies in multijunction designs.

In addition to spectral control, QDs exhibit extremely high absorption coefficients—often exceeding those of bulk semiconductors by an order of magnitude—which allows them to absorb most incident light within just a few hundred nanometers of material (Brus, 2020). This makes them ideal candidates for thin-film, flexible, and lightweight photovoltaic applications. Moreover, their capacity to support multiple exciton generation under high-energy photon excitation introduces further opportunities to surpass traditional efficiency limits.

The optoelectronic behavior of QDs depends heavily on the underlying material. For instance, PbS and PbSe are often chosen for their infrared absorption and suitability for MEG, while CdSe offers efficient visible light absorption. More environmentally benign options, including indium phosphide (InP), copper indium sulfide (CuInS), and carbon-based QDs, are actively being developed to address toxicity concerns. Each of these materials presents trade-offs in terms of quantum yield, stability, and compatibility with device architectures. A comparative overview of their key properties—including bandgap ranges, absorption behavior, and environmental profiles—clarifies their strengths and limitations in photovoltaic contexts.

Synthesis methods such as hot-injection, solvothermal, and microwave-assisted techniques allow researchers to

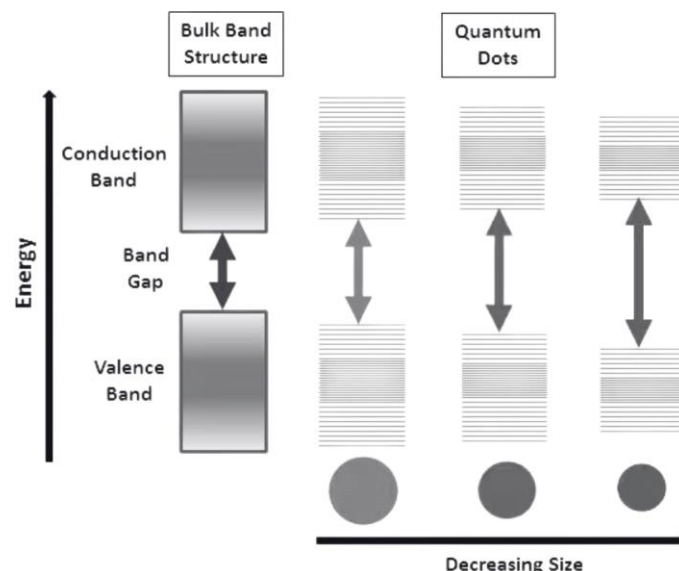


Figure 1: Schematic comparison of the electronic band structure in a bulk semiconductor (left) and quantum dots (right) of decreasing size.

In bulk materials, continuous energy bands define a fixed bandgap between the conduction and valence bands. In quantum dots, quantum confinement leads to discrete energy levels, and as the dot size decreases, the bandgap widens. This size-dependent tunability enables spectral control of absorption properties, which is crucial for optimizing light harvesting in photovoltaic applications.

finely tune QD size and composition, thus controlling their electronic and optical characteristics (Koh et al., 2018). These colloidal routes also allow for surface functionalization, though the long-chain ligands used during synthesis can hinder charge transport in solid films. As a result, post-synthesis ligand exchange is commonly employed to improve inter-dot coupling, albeit with trade-offs in surface passivation. Engineering strategies such as core-shell structures and halide treatments are often applied to reduce surface trap densities and enhance photostability .

Ultimately, differences in particle size, structure, and surface chemistry are what define the utility of QDs in solar energy applications. A broad understanding of these materials sets the stage for identifying specific physical mechanisms—such as carrier multiplication and energy transfer—that influence the performance of QD-based photovoltaic systems.

Table 1: Comparison of key quantum dot materials used in solar cells, summarizing their bandgap ranges, absorption characteristics, toxicity, and stability.

Material	Bandgap Range (eV)	Absorption Range	Toxicity	Stability	Notes
CdSe	1.7–2.4	Visible	High	Moderate	High PLQY, well-studied
PbS	0.7–1.5	Near-IR	High	Moderate	MEG potential, tunable IR
InP	1.3–1.9	Visible–NIR	Low	Fair	Eco-friendly, lower PLQY
CsPbBr ₃	2.1	Visible	Medium	Improving	Perovskite QD, high efficiency
CuInS ₂	1.5–1.6	Visible–NIR	Low	Good	Lower toxicity, low cost
Carbon QDs	~2.0–3.0	UV–Visible	Non-toxic	High	Poor charge mobility, emerging class

While CdSe and PbS offer high efficiency and MEG potential, their toxicity limits large-scale adoption. Low-toxicity options like InP, CuInS₂, and carbon QDs are safer but

usually less effective. Material choice significantly impacts photovoltaic efficiency and environmental sustainability.

2– Key Physical Phenomena in QD–Based Solar Cells

One of the most interesting things about quantum dots (QDs) is that they can produce more than one exciton from a single photon. The energy of a photon produces only one electron–hole pair in most solar cells; the extra energy is lost as heat. But by tapping into that extra energy, QDs can generate more excitons. This leads to the generation of more charge carriers, which increases the current of the device (Beard et al., 2014). Due to their discrete energy levels and strong Coulomb coupling, QDs result in less heating and allow to produce more charges.

The photon energy should be twice the energy of QD bandgap to create multiple excitons. The surplus energy is afterwards rapidly dissipated, forming Ground State in multiple excitons. This so–called multiple exciton generation (MEG) has already been demonstrated by researchers in the case of QDs such as PbSe and PbS. However, the composition of the material, the roughness of the surface and extensive preparation, and other factors such as losses to non–radiative processes, especially to Auger recombination, also regulate how effectively MEG works. We have shown that quantum dots (QDs) can sometimes reach external quantum efficiencies higher than 100% when they are exposed to the right kind of light (Brennan et al., 2020). This means that a single photon can make more than one electron–hole pair, which is not possible with regular materials. and this shows the unique advantages of QDs and how they could make solar cells work better in the future.

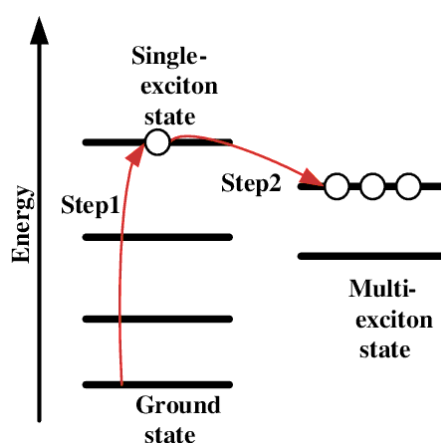


Figure 2: This diagram shows how the process of Multiple Exciton Generation (MEG) works inside a quantum dot.

In the first step, a high-energy photon hits the quantum dot and creates one exciton (an electron-hole pair). However, in Step 2, the quantum dot uses the excess energy to create more excitons rather than allowing it to be converted to heat as is the case in conventional semiconductors. This implies that multiple electron-hole pairs can be created by a single photon. As a result, the solar cell has more charge carriers, which can enhance its functionality. Indeed, this procedure may enable solar cells to achieve efficiencies above the Shockley-Queisser limit.

The construction of quantum dot solar cells (QDSCs) makes it challenging to move and collect charge carriers. They rely on nanocrystals, ultra-fine crystals linked through inorganic or organic substances. Such current carrying capability will deteriorate, with recombination losses increasing, if these contact interfaces are weaker or in mismatch (Kovalenko et al., 2020). A common way for researchers to address this is by replacing long, insulating connectors with shorter, more electrically conductive ones. They still need to keep the stability and barrier properties of the surface (Koh et al., 2018).

The recombination of charges is also impacted by QD surfaces. QDs tend to be riddled with microscopic surface defects owing to their very high surface-to-volume ratio. These defects can lead to energy loss by non-radiative recombination. One way of mitigating this is with 'shells' or caps by enveloping the whole CdSe inside for instance a coat of ZnS, or treating it with halides. But there are problems with keeping the device stable and working well in low light. Another important part is making sure that the energy levels of the quantum dots are in line with those of the nearby charge transport layers. If the energy levels aren't lined up correctly, charges may have a harder time moving or recombining at the interface, which would make the device work less well. To fix this, scientists can use better transport materials, add more layers to help with energy alignment, or change the size or makeup of the quantum dots. Some of the ideas that define the limits and potential of quantum dot solar cells are multiple exciton generation (MEG), smooth charge transport, surface defect control, and good energy alignment. You need to know how quantum dots work in order to make better solar devices that use them to their full potential.

3- Quantum Dot Solar Cell Architectures

How quantum dots (QDs) are fabricated and structured relates to how effective they are in their use in solar cells. In the field of solar technology, quantum dots (QDs) serve in various roles including as components in quantum dot solar cells (QDSCs), quantum dot

heterojunction cells, as well as in tandem cells containing quantum dots in the light absorbing layers. Each subtype of QD solar cell tries to improve on the same basic aspects: light absorption, charge separation, and charge transport.

In QDSCs, quantum dots are deposited onto porous substrates like ZnO or TiO₂ which serve as charge collectors and transporters. These materials facilitate electron transport. In the CUROD system, as light is absorbed by the quantum dots, electrons are ejected into the conduction band of the oxide. At the same time, a liquid electrolyte occupies the voids in the system.

This design is akin to some older dye-sensitized solar cells and is relatively straightforward. Additionally, this design captures broad excitation spectra. Its main drawback stems from using liquid electrolytes, which tend to be unstable over time and impact the device's overall longevity. Rather than flowing freely, electrons get stuck within the liquid electrolyte.

Unlike other QDSCs, heterojunction QDSCs stand out because their entire composition consists of solids. This type of solar cell has a QD layer positioned between two solid layers. One layer is a hole transport layer and the other is an electron transport layer. Solar radiation can be absorbed by quantum dots such as PbS or InP. Electrons get collected by ZnO or TiO₂, while holes are collected by Spiro-OMeTAD or MoO₃. This approach has large scale production advantages as it does not require water, but these solid cells have their own issues. For example, the QDs may have insufficient charge mobility, and there may be poor interfacial layer alignment which could diminish device performance.

The capability of QDs to have their bandgap adjusted enables the use of silicon and perovskite with tandem solar cells. QDs can be placed on either the upper or lower regions of the solar cells to utilize portions of sunlight. Stacking layers capable of harnessing different portions of the light spectrum is designed to improve efficiency beyond a single-junction solar cell (Green et al., 2014). For example, the device captures more sunlight by using PbS QDs to capture near-infrared light and then placing a perovskite layer on top to capture higher energy light.

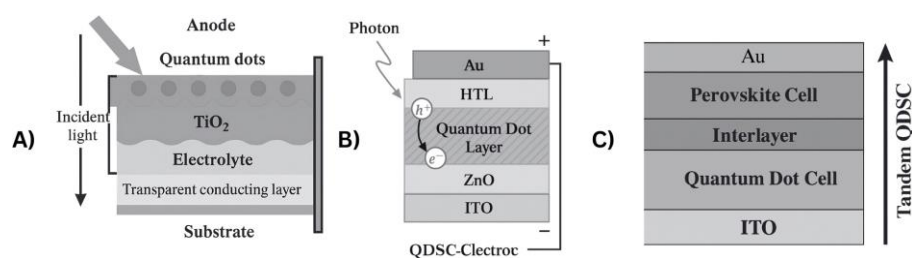


Figure 3: Comparison Figure 3 shows three main types of quantum dot solar cell (QDSC) designs.

(a) The QD-Sensitized Solar Cell (QDSSC) uses quantum dots as sensitizers placed on a mesoporous oxide. It pulls charge carriers through a redox electrolyte. (b) The Heterojunction QDSC has a solid-state junction where quantum dots connect with electron and hole transport layers. (c) The Tandem QDSC combines quantum dots with perovskite or other top cells. This design improves light absorption by allowing different wavelengths of light to be used more effectively.

Actual performance metrics and efficiencies demonstrate the effectiveness of these structures and designs. Some values, like current density, open-circuit voltage, and efficiency are influenced by the type and preparation method of the QD used. Solar cells containing CdSe, PbS, InP, and perovskite quantum dots are summarized with their corresponding metrics in Table 2.

The data shows that there isn't one best design for every category. Quantum dot solar cells (QDSSCs) allow for broad tuning of light absorption and are easy to make, but their liquid components limit their long-term use. Heterojunction cells are more stable but require careful engineering to ensure efficient carrier extraction. Tandem devices offer the highest potential efficiency but face challenges in manufacturing complexity, matching light absorption, and reducing losses between layers.

Table 2: Representative photovoltaic performance metrics for selected quantum dot materials and device architectures.

QD Material	Architecture	Voc (V)	Jsc (mA/cm ²)	FF	PCE (%)
PbS	Heterojunction	0.56	21.2	0.71	8.4
CdSe	Sensitized (QDSSC)	0.55	15.2	0.53	4.5
InP	Heterojunction	0.59	17.8	0.52	5.4
CsPbBr ₃	Tandem (with Perovskite)	1.05	18.3	0.74	16.4
CuInS ₂	Sensitized	0.58	14.0	0.55	4.3

Values include open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency (PCE), illustrating trade-offs in efficiency across sensitized, heterojunction, and tandem designs.

4- Challenges and Limitations

Quantum dot solar cells (QDSCs) have a lot of potential, but there are a number of problems that make it hard for them to be used widely. Some of these problems are toxicity, how well the charge moves, how stable the material is, and how hard it is to make things on a large scale. Stability is one of the most important things to think about. Quantum dots (QDs) can be affected by changes in temperature, oxygen, and moisture. When lead sulfide (PbS) and perovskite QDs come into contact with air or moisture, they can break down, which makes them less useful. There have been some improvements in the use of protective layers and coatings to make QD-based solar devices more stable, but most of them still don't last as long as regular silicon or thin-film solar cells. Toxicology is another big problem. Heavy metals like lead (Pb) and cadmium (Cd), which are against environmental laws like RoHS and REACH, are used to make some of the best quantum dots. People and the environment could be harmed if these metals leak during production, use, or disposal. Researchers are trying to find safer options, such as carbon dots, copper indium sulfide (CuInS₂), and indium phosphide (InP). But these materials aren't as stable or effective as the ones that are more toxic.

Another issue is that quantum dot (QD) solids don't do a good job of moving charges. This happens because the links between the nanocrystals aren't perfect, and there are small energy gaps between them. The long organic ligands that are used to make them can also act as insulators and keep charges from moving. Using shorter or inorganic ligands can help charges move and make connections better. But this can also make the surface weaker and add more places where charges can get stuck, which makes recombination happen. Also, if the energy levels of the QDs don't match up well with the transport layers around them, it becomes harder for charges to separate, and more energy may be lost at the interface.

Making a lot of QDs while keeping their quality the same is also very hard. Colloidal chemistry lets scientists make a lot of QDs at once, but it's still hard to make films that are smooth and free of defects over large areas. Some lab methods, like spin coating or layer-by-layer assembly, work well, but they are too slow and not reliable enough for use in industry. Newer

methods like roll-to-roll processing, spray coating, and inkjet printing look promising, but they can make films that aren't even, which could make the solar cells work less well overall.

It is not easy to always ensure the uniformity of QD samples. Even factors such as the reaction time, temperature, or even the materials used can significantly affect the surface properties and the size of the QDs. These discrepancies alter the functionality of the QDs, posing challenges when trying to develop robust and reliable devices. These challenges illustrate the gap that continues to exist between the remarkable attributes of QDs at the nanoscale and the difficulties associated with their integration into real-world applications. Bridging this gap will require an interdisciplinary approach embracing environmental science, device design, surface chemistry, and large-scale manufacturing.

5- Future Directions

In order to improve the performance of quantum dot solar cells, we have to enhance the materials, fabrication, and scaling-up processes. Today, these QDSCs suffer from several problems, such as poor charge transport, instability, and toxicity. However, other researchers are looking to address these problems. Safer and more abundant alternatives to QDs are being developed, which substitute lead or cadmium containing QDs. Suitable candidates include carbon dots, copper indium sulfide (CuInS₂), and indium phosphide (InP). To optimize the performance of such new materials, scientists employ doping, core-shell structure fabrication, and alloying—the process of mixing different materials. These approaches aim to preserve the favorable characteristics of older QDs, while making them more environmentally benign and non-toxic.

It is also fascinating to consider tandem solar cells with QDs used as sub-absorbers since this design has the potential to surpass the Shockley-Queisser limit. QDs have the ability to absorb near infrared or ultraviolet light which is compatible with top layers like perovskites and silicon.

Flexible and wearable photovoltaics represent a compelling application area for QDs, given their solution processability and compatibility with low-temperature fabrication on plastic or metal foils. QD-based films can be incorporated into lightweight, conformable devices for use in portable electronics, biomedical sensors, and off-grid energy systems. However, ensuring mechanical durability and environmental stability under bending, humidity, and UV exposure remains a key research priority.

Scalable manufacturing techniques, such as inkjet printing, spray coating, and roll-to-roll deposition, are under development to enable high-throughput QDSC production. These methods must be coupled with innovations in film morphology control, ligand engineering, and device encapsulation to preserve efficiency while reducing cost and material waste.

AI and machine learning are increasingly being used to accelerate quantum dot design and optimization. Predictive algorithms can model synthetic conditions, forecast optoelectronic properties, and screen ligand combinations more efficiently than conventional trial-and-error approaches. This data-driven methodology could significantly shorten the discovery cycle for high-performance, non-toxic QDs.

Advanced QD structures, like gradient core-shells, alloyed nanocrystals, and Janus heterostructures, are being developed to reduce non-radiative recombination, improve carrier separation, and extend lifetimes. These innovations could achieve performance and stability improvements beyond conventional spherical QDs.

Ultimately, realizing the full potential of QD photovoltaics will require synergistic progress across material chemistry, device physics, environmental science, and industrial processing. Equally important will be establishing robust life cycle analyses, toxicity assessments, and standardization protocols to ensure safe and sustainable deployment. Collaborative efforts between academia, industry, and policy makers will be essential in translating laboratory breakthroughs into commercial reality.

Conclusion

Quantum dots (QDs) offer a highly tunable platform for next-generation photovoltaics, thanks to their size-dependent bandgaps, high absorption coefficients, and potential for multiple exciton generation. This review has highlighted their fundamental properties, key mechanisms, and integration into various solar cell architectures.

While challenges remain—particularly regarding toxicity, stability, and charge transport—advances in eco-friendly materials, surface engineering, and scalable processing are steadily closing the gap toward practical deployment. Emerging approaches like tandem designs, flexible substrates, and AI-driven optimization further expand the potential of QD solar technologies. With continued interdisciplinary progress, QDs are poised to play a central role in developing efficient, low-cost, and sustainable solar energy solutions.

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