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Next-generation quantum dot solar cells: advances in materials, device engineering and performance optimization

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Quantum dot solar cells (QDSCs) have emerged as promising next-generation photovoltaic technologies owing to their tunable bandgaps, strong light absorption, solution-processability and potential to surpass the Shockley–Queisser efficiency limit through multiple exciton generation (MEG). This review presents a comprehensive and critically structured overview of recent advances in QDSCs by integrating material development, device engineering, interface optimization, and stability enhancement strategies within a unified framework. Unlike previous reviews that primarily focus on individual material systems or device architectures, this work systematically correlates quantum dot absorber materials, electron and hole transport layers, electrode engineering, fabrication methodologies, and charge-transfer mechanisms with photovoltaic performance metrics. Emphasis is placed on the comparative analysis of PbS, CdSe, perovskite, graphene and environmentally benign quantum dots, highlighting their influence on efficiency, charge transport, stability, and scalability. In addition, recent developments in interface engineering, ligand exchange, surface passivation, core–shell structures, plasmonic enhancement, and hybrid architectures are critically discussed as key routes for suppressing recombination losses and improving long-term operational stability. Emerging trends including AI-assisted device optimization, tandem configurations, and environmentally sustainable QD materials are further evaluated to identify future commercialization pathways. Despite significant progress, challenges associated with toxicity, large-scale fabrication, and environmental stability continue to limit practical deployment. Overall, this review provides a comparative and future-oriented perspective that bridges materials science, device physics, and scalable engineering approaches, offering strategic insights for the development of efficient, stable, and commercially viable QDSCs for next-generation solar energy technologies.

1. Introduction

Recent advances in solar photovoltaic (PV) technologies have revolutionized the sphere of renewable energy. Solar photovoltaic systems which convert sunlight into electricity with the direct conversion of semiconductor materials have evolved greatly since their inception. Through these advancements, solar energy has become a more viable and competitive energy source as compared to the traditional sources of energy since materials have been refined to increase their efficiency and application.[1] The problem of effective, sustainable energy solutions is urgent because the energy consumption rates of the world are growing, and the consequences of climate changes become more evident. Increased PV efficiency enables the generation of more energy with the same amount of sunshine that directly translates into better performance and cost-effectiveness. Improvement in materials like development of new semiconductors and new coatings has also resulted in PV systems that are more durable and have greater ability to convert energy. Moreover, various applications have led to the growth in uses of solar PV even in several industries with an application in building materials and off grid solution.[2]

Solar energy is one of the critical alternatives to fossil fuels in the quest to have sustainable power and therefore it is taking the lead in the global shift to renewable energy.[3] Although effective, the traditional photovoltaic (PV) technologies have limitations like limited flexibility, expensive materials and performance issues. Since there are now bifacial panels that can generate more energy up to 30% and solar cells employing multiple junctions with efficiencies reaching almost 40% when using concentrated sunlight, it can be seen that solar technologies have developed very quickly. However, the development of

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solar cell efficiency, cost reduction and flexibility in design is still an ongoing trend in materials science and optimization of designs of solar cells.[4] Solar cells have passed through a number of generations in terms of material composition, methods of their fabrication, and their efficiency levels. The oldest and the most common technology considered is the first-generation solar cells which are monocrystalline and multi crystalline silicon cells. The thin-film technologies of CdSe and Cu(In,Ga)Se_2 used in the production of second-generation are predominant, using less material and having low manufacturing costs. The third-generation solar cells feature dye-sensitized (DSSCs) as well as organic (OSCs) solar cells, perovskite solar cells and quantum dot solar cells (QDSCs) are new technologies that aim to combine high efficiency with low-cost, mechanical flexibility, and optical transparency. The rise of the new solar cell technologies can be seen in Fig. 1 that shows the developmental route of the advanced photovoltaic systems using the semiconductor materials.[5]

The solar cells can convert the incidence sunlight into electrical energy. High efficiency, long-term stability and cost-effectiveness are among the attributes that have propelled the fast development in solar cell research and development. This has led to the introduction of several solar cell designs in high-performance that would be made using other semiconductor materials. Presently the commercial solar sector is dominated by silicon solar cells, III 5 V compound solar cells (including GaAs) and thin-film technologies in terms of Cu(In,Ga)Se_2.[6,7] Nevertheless, these traditional technologies have been challenged in the aspect of cost, rigidity and efficiency constraints. Since solar cells can harness solar power, it has offered remedies to energy crisis and pollution of the environment. Emissions of carbon dioxide by traditional energy sources contribute to the situation of worsening the greenhouse effect, and solar technology can be a viable and clean substitute. On-going attempts to become out of the constraints of conventional solar cells have seen the emergence of sophisticated and intricate photovoltaic architectures. Among third-generation photovoltaic technologies, QDSCs have emerged as particularly promising candidates owing to their unique optoelectronic properties, and are the primary focus of this review with regard to their design, working principles, fabrication, simulation, and mathematical modelling.[5]

A quantum dot (QD) is a size-dependent electrical and optical nanoparticle with a diameter of 2–10 nm in size that is produced by quantum confinement effects in a semiconductor nanoparticle.[8] QDSCs are a type of photovoltaic technology,[9] which uses quantum dots as a light-absorbing material. In contrast to bulk semiconductors, quantum dots are size-tunable, which means that their bandgaps can be closely controlled and that they absorb a wide portion of the solar observed spectrum, including ultraviolet and infrared radiation.[10,11] Fig. 2 represents the quantum constraint effects in semiconductors. In bulk semiconductors continuous bands of valence and conduction bands are observed with a fixed bandgap. Conversely, due to carrier confinement in three dimensions, QDs have discrete energy levels. The effective bandgap would increase to produce size-dependent optical and electrical behaviour when the QDs size is decreased to the point where the exciton Bohr radius is lower than the dot size.[12]

QDSCs have become an important breakthrough in photovoltaic technology since it is a solution to several drawbacks of traditional solar cells. With their high light absorptivity, their multiple exciton generation (MEG) capability enables theoretical efficiencies superior to the Shockley–Queisser limit. With

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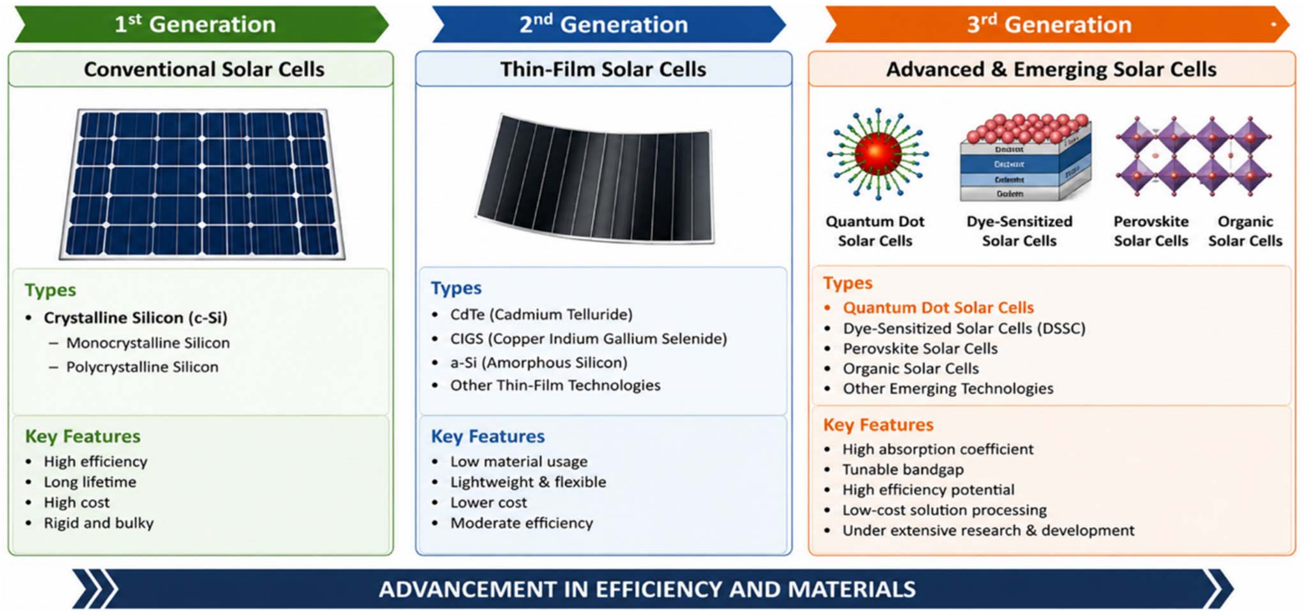

Fig. 1 Evolution of solar cell technologies across generations.[5]

QDSCs, one intense photon can create multiple pairs of electrons and holes so that conversion of energy can be highly efficient.[11] Moreover, spin-coating, dip-coating, and doctor-blading, which are employable in fabrication of solutions, are cost-effective and can be scaled to substitute traditional silicon process technologies.[4] Spin-coating, among others, is one of the methods that lower costs of production of both QDSCs and silicon. Much higher efficiencies of up to 18.1% have been achieved by using advanced ligand-exchange strategies that eliminate defects and enhance stability, to realize perovskite

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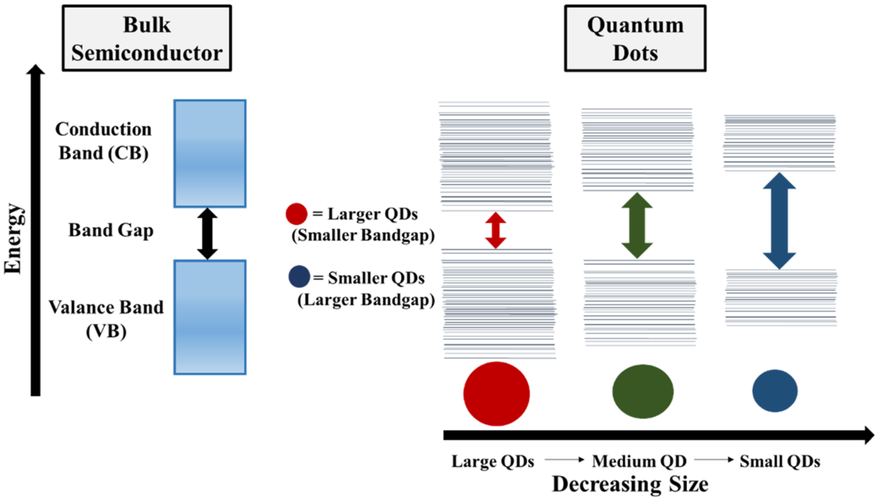


Fig. 2 Representation of quantum constraint effects in semiconductors.[12]

Table 1 Summary of representative high-performance QDSC material systems and their reported photovoltaic parameters

QD material	Device architecture	Certified PCE (%)	Key strategy	Stability	References
$CsPbI_3$ perovskite QDs	Depleted heterojunction	16.6	Ligand exchange; iodide treatment	Moderate; moisture sensitive	15
$CsPbI_3$ perovskite QDs	Hybrid/tandem	18.1	Surface passivation; advanced ligand exchange	Moderate; encapsulation required	16
Perovskite QDs (certified)	Hybrid/tandem	18.3	Alkaline capping treatment; conductive capping enrichment	Improving; encapsulation extends lifetime	14
PbS QDs	Depleted heterojunction	13.8	Triple cation passivation; ZnO ETM	Good; >1200 h shelf stability	17
ZCISSe QDs	Sensitized QDSSC	15.31	Secondary QD deposition; CLIS strategy	Moderate; electrolyte instability	18
$CuInS_2$ QDs	Sensitized QDSSC	∼4–7	ZnS shell passivation; thiourea treatment	Good; Pb/Cd-free system	19
Carbon QDs	Flexible QDSSC	∼3–6	N-doping; co-sensitization with N719 dye	Excellent; photostable in ambient conditions	20
Sn:InP QDs	Sensitized QDSSC	3.54	Sn doping; improved TiO_2 band alignment	Good; lead- and cadmium-free	21

quantum dot devices.[13] Notably, rapid progress over the past five years has pushed QDSC efficiencies significantly forward, with certified power conversion efficiencies (PCEs) rising from approximately 13.4% in 2022 to a record 18.3% reported for perovskite QD-based devices in 2025 by Jia *et al.*[14] The rapid progress in QDSC efficiency over the past five years is best understood through a chronological and material-specific lens. Multiple efficiency values cited across the literature including 16.6%, 18.1%, 18.3% and 18.24% refer to distinct material systems, device architectures, and reporting years, and should not be interpreted as contradictory. Table 1 systematically organizes these values to provide a clear and comprehensive overview of efficiency milestones achieved across different QD material systems from 2020 to 2025.

As evident from Table 1, perovskite QD-based devices have demonstrated the highest certified PCEs, progressing from 16.6% in 2020 to 18.3% in 2025. It is important to note that the value of 18.24% reported in this review refers specifically to a perovskite thin-film device employing a hybrid TiO_2/ZnO electron transport layer and is therefore not directly comparable to standalone QDSC records. In contrast, environmentally benign alternatives such as $CuInS_2$ and Sn:InP QDs currently achieve lower PCEs of 4–7% and 3.54% respectively, but offer superior toxicity profiles and represent important parallel research directions for sustainable photovoltaic development. Table 1 systematically organizes all efficiency values cited in this review to avoid confusion arising from scattered data presentation. Despite this remarkable progress, a substantial gap remains between the current experimental efficiency ceiling (∼18.3%) and the theoretical maximum efficiency predicted for QDSCs through multiple exciton generation (∼66%), as well as the intermediate band concept (∼44.7%), underscoring the significant room for further improvement and the urgent need for continued materials innovation, interface engineering, and device optimization, as shown in Fig. 3.[22,23] In multilayer QDSC module, it is the hole transport layer, which acts as a redox

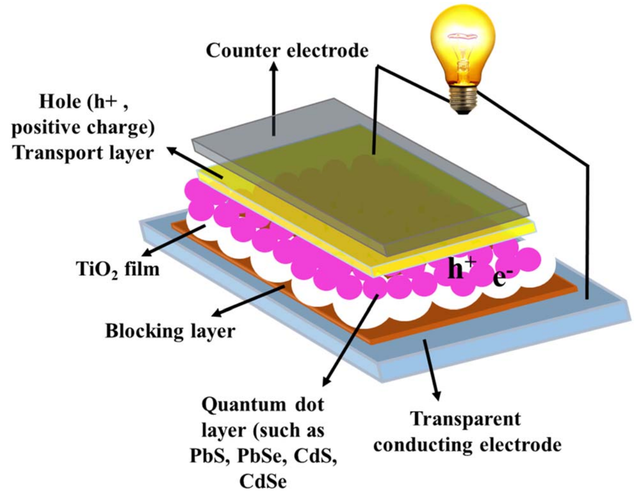


Fig. 3 QDSC anatomy showing the various layers.[24]

electrolyte in liquid-junction module, or a transport layer in heterojunction designs. The core of the photoactive region consists of an active mass in the form of an active layer of quantum dots of approximately 0.25 cm^2 which is sandwiched between the OTE and the redox electrolyte.[11,12]

QDSCs have demonstrated significant potential as a high-performance solar energy technology, with recent findings providing compelling evidence for their commercial viability. This review assesses novel semiconductor QD systems with respect to their stability, scalability, and photovoltaic performance, while addressing commercialization challenges including environmental stability, toxicity, and large-scale fabrication. This review synthesizes current strategies for addressing existing challenges and provides directions for accelerating the commercialization of QDSC technology.[5] A concise conclusions and future outlook section is also provided to guide next-generation QDSC research. The bandgaps of quantum dots are precisely tunable through size control, enabling broad spectral absorption across ultraviolet to near-infrared wavelengths. QD absorbers operate with high absorption coefficients even in ultrathin active layers. Quantum dots (QDs) have a potential to overcome the Shockley–Queisser efficiency limit since one high energy photon can create multiple excitons in multiple exciton generation (MEG).[25] In solar cell designs, the QDs are commonly used as light absorbing material, where they replace the dye molecules in the dye-sensitized solar cells (DSSCs), serving as the sensitizer. This was usually achieved by coating these QDs on a mesoporous scaffold, usually TiO_2, which allows the separation of charges, and the resulting electron–hole pair undergoes charge transfer with the redox electrolyte solution.[26] The integration of the QDs with organic polymers can produce bulk heterojunction structures improving charge separation and improving the efficiency of charge transport.[27] In addition, QDs have intermediate energy levels, which allow absorption of sub-bandgap photon to enhance the overall light-harvesting ability.[28] The production of a pair of QD solar cells involves thriving numerous types of semiconductor materials where PbS quantum dots and materials have received a lot of research focus owing to its high near-infrared absorbency. Moreover, II–VI semiconductor QDs have tunable bandgaps at the visible spectral range, which is very flexible to optoelectronic applications.[29] $CuInS_2$ QDs possess favourable optical properties and low toxicity, making them highly suitable for sustainable solar cell applications. Perovskite QDs represent materials that have intense potential in the application of solar cells since they have got very unique optoelectronic skills and easy to use synthetic technology.[30] Graphene quantum dots (GQDs), as zero-dimensional carbon nanomaterials, have also been explored as sensitizers in QDSSCs owing to their tunable electronic properties and chemical stability.[25] Precise control over the size, shape, and surface chemistry of QDs is achieved through colloidal synthesis procedures. Surface engineering through ligand modification remains critical for passivating QD surface defects and enhancing device stability and photovoltaic performance.[31]

QDSCs offer several significant advantages over traditional solar cell technologies, including MEG, adjustable bandgaps, and broad spectral absorption. In addition, QDs can be synthesized at low cost *via* solution-based methods that are compatible with large-scale production.[32] The compatibility of QDSCs with flexible substrates further expands their applicability to wearable, portable, and building-integrated photovoltaic systems.[33] Despite the considerable promise of QDSCs, several challenges remain. Environmental variables also affect PQDs and other QDs, reducing their operational capability for deterioration.[28] Since lead and cadmium are hazardous to ecosystems, their QDs pose a harm to the environment as well. For the QD layer and the electrode contact to function well, better charge transport is required.[26] Although research has shown increasing efficiencies, the efficiency rate cell technology is still lagging behind both silicon cells and PSCs.[34] Future research directions include developing stable QD device designs, enhancing charge transport and collection efficiency, exploring novel material combinations, and exploiting the plasmonic properties of metal nanoparticles to further improve photovoltaic performance.[35] Addressing these challenges is essential to establish QDSCs as an efficient, cost-effective, and sustainable renewable energy technology.[36]

Fig. 4 shows how QDs have numerous and important applications in both science and the majority of technological fields. QDSCs use QD particles to convert sunlight into energy at a high efficiency. The QDs have unique benefits such as tunable bandgaps, multiple exciton generation (MEG), and wide spectral absorption, which theoretically enable potential efficiencies exceeding 66%, though the highest certified efficiency reported for modern QDSC devices has reached 18.3% as of 2025.[14] The solution-processable nature of QDs makes them lightweight, mechanically flexible, and cost-effective to manufacture, rendering them highly suitable for emerging applications including wearable electronics, building-integrated photovoltaics (BIPV), and flexible portable energy systems. With these advantages there are still difficulties in that it has environmental concerns, material degradation and low stability in moisture or heat. To overcome these problems and increase stability and performance, the scientists consider the following

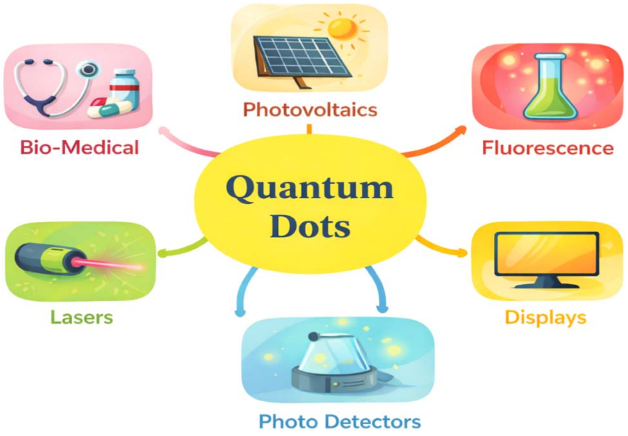


Fig. 4 Applications for quantum dots.[39,40]

strategies, including perovskite-based integration, core–shell nanostructures, superior surface passivation, and optimization with the help of artificial intelligence. As safer and more sustainable material advances continue to be made, more advanced QDSCs are also considered to be good candidates of scalable solar energy technologies.[4] Recent advances have also expanded the application of quantum dots toward luminescent solar concentrators (LSCs), which are emerging as promising technologies for building-integrated photovoltaics and semi-transparent solar harvesting systems. In particular, carbon dots, perovskite quantum dots, and environmentally benign semiconductor QDs have demonstrated enhanced photoluminescence efficiency, large Stokes shifts, and improved optical wave guiding properties suitable for next-generation LSC devices. Recent studies published during 2024–2025 have highlighted the growing potential of QD-based LSCs for scalable and energy-efficient photovoltaic applications.[37,38]

This article presents a comprehensive overview of recent advancements in QDSCs, covering working principles, material systems, device architectures, performance optimization strategies, and future research directions. By critically reviewing existing advances and persistent challenges, this review aims to provide useful insights toward the development of efficient, reliable, and commercially feasible QDSC technologies. This review provides a comprehensive overview of recent advances in QDSCs, including quantum dot materials, device architectures, charge transport mechanisms, mathematical modelling, and performance optimization strategies. Particular emphasis is placed on recent progress in efficiency enhancement, interfacial engineering, stability improvement, and scalable fabrication approaches. By critically evaluating current achievements and remaining challenges, this review aims to provide valuable insights for the future development of efficient, stable, and commercially viable QDSC technologies.

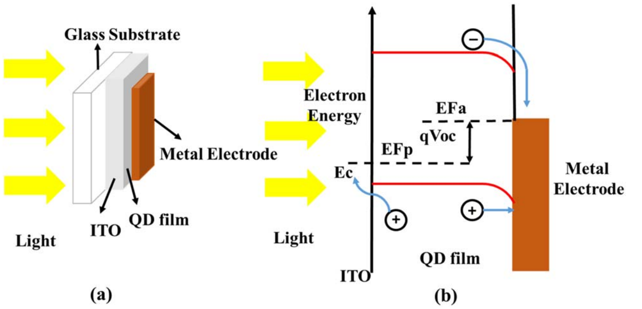


Fig. 5 (a) A quantum dot-based solar cell system, (b) band diagram for solar cells.[43]

2. Fundamental principles of QDSCs

Quantum dot solar cells (QDSCs), also referred to as nanocrystalline solar cells, utilize semiconductor QDs as the primary light-absorbing material. Unlike bulk semiconductors, QDs can be grown epitaxially on crystalline substrates or synthesized *via* colloidal methods, offering precise control over their optoelectronic properties. The small size being nanoscale size constraints charge carriers on all three space directions in high potential barriers, consequently, discrete energy states exist; therefore, ground-state energy of the electrons and holes is highly dependent on the size of the dots.[41] Solar cells that have a nano crystalline structure also possess extremely high absorption coefficient. The photovoltaic process usually uses four consecutive stages, which would be: (1) absorption of light and creation of exciton, (2) diffusion of exciton, (3) charge separation, and the fourth stage of charge conduction. In organic materials, short exciton diffusion lengths (proximate to 1020 nm) can be brought about by the restricted mobility and short lifetimes of excitons, thus recombination losses due to exciton generation away from the charge–collection interfaces can be brought about, thereby diminishing conversion efficiency.[42] The onset of metal halide perovskite thin-film solar cells has added to growing interest in the use of QDs and nanocrystals as diverse photovoltaic materials. Recent developments in mixed colloidal perovskite QDs have pushed QDSC efficiencies to a certified record of 18.3% as of 2025.[14] These nanomaterials are also extremely versatile due to their simple fabrication, tunable bandgaps and controllable surface chemistry which allow them to be designed into many different devices, including single-junction, semitransparent, flexible, heterostructure, and tandem solar cells. The reduction of QD size distribution can also increase device performance, smaller dots can have better electron transport characteristics because of reduced band-tail states, and the bandgap of QDs near the contacts affects the open-circuit voltage (V_{oc}) and the overall device efficiency.[41] By reducing these losses, increasing QD size homogeneity and uniformity would also improve PV performance. Even though the reported controlled experiments like this have yet to be done, there is potential that additional controlled synthesis may have benefit in QD cells.[42] The structural and band alignment representation shown in Fig. 5 provides additional evidence for these basic processes.

2.1. Design and working principle of quantum dot-based solar cells

QDs are the primary light-absorbing component of QDSCs, which acts as a good photon converter to convert solar energy

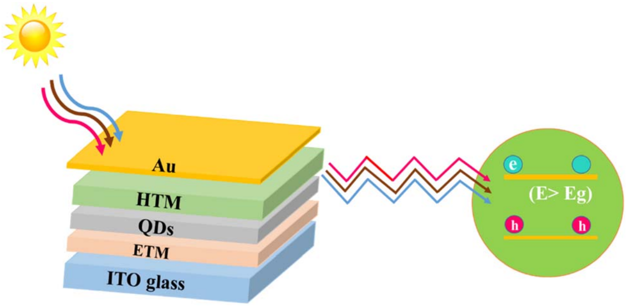


Fig. 6 Diagrammatic representation of a QDSC.[5]

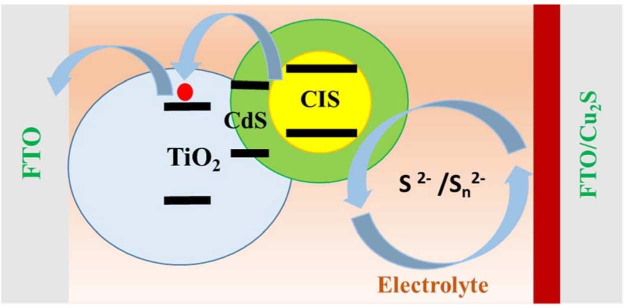


Fig. 7 Diagrammatic representation of the electrical mechanisms and architectures of the QDSSCs put together with CIS/CdS core/shell QDs.[48]

into an electric signal. When photons with energy equal to or greater than a QDs bandgap absorb photons, one electron is excited from the valence band into the conduction band, creating an exciton and an excited electronic state in the QD. Quantum confinement allows regulating the size of QDs to achieve overall emission color shifting of quantum modes, scaled by the size of QDs, a wide spectral range capture, and harsher light utilization, leading to higher photovoltaic efficiency.[44] The separation and transmission of photogenerated electrons and holes to the appropriate electrodes in order to produce a photocurrent is the second most crucial step in QDSC operation, following the excitons creation.[45] QDSCs use charge separation on the basis of positive energy-level consistency between the QDs and any adjacent layer of the charge-transport selectively. Electrons are also transported immediately to the conduction band of the QDs to the electron transport material (ETM), which is usually TiO$_2$ or ZnO, and holes are transported to the electrolyte or holes transport material (HTM).[46] Because the separation and transit efficiency of the carriers generated during the photo production process are important factors affecting the overall performance of QDSC-based devices, it is imperative to disperse charge effectively and efficiently in order to limit the amount of recombination losses.[47] Fig. 6 shows the entire light absorption, carrier separation, and transport mechanism inside the QDSC design.

The QDSSC is one of the architectures of QDs scratchable surfaces on mesoporous TiO$_2$ oxide films. A typical QDSSC typically consists of a photo anode composed of a counter electrode, an electrolyte, and a QD-sensitized mesoporous wide-bandgap semiconductor. Upon light excitation, electrons in the QDs are promoted from the valence band to the conduction band and travel through efficient charge transport pathways to be extracted at the electrode.[48] The electrons injected pass to TiO$_2$ through the system of the electrode and on to the transparent conducting electrode comprising of FTO, or ITO, and then pass on *via* the external circuit. At the same time, the oxidized QDs can be reduced by a redox electrolyte (typically a polysulfide), which takes electrons off the other electrode and closes the electrical circuit as shown in Fig. 7.[49]

In general, QDSC performance is governed by the interplay of QD bandgap, light absorption properties, surface defect concentration, and charge carrier transport efficiency.[13] Surface defects in QDs may serve as non-radiative centers resulting in a significant loss of charge; thus, surface passivation schemes containing inorganic coatings or ligand exchange are typically utilized in order to improve the charge transport and cast off recombination. The interface between the ETM and HTM critically determines charge collection efficiency, while optical management strategies such as Fabry–Perot resonators can further enhance light harvesting in the active layer.[49] Furthermore, as shown in Fig. 8,[50] optimized QD loading on TiO$_2$ sheets improves light absorption and charge production.

2.2. Synthesis strategies for QDs

QD synthesis is broadly classified into two approaches: top-down and bottom-up. The top-down approach involves breaking down bulk materials into nanoscale particles, which are produced by processing methods that include: reactive ion etching, focused ion beam processing and wet chemically etching (Fig. 9).

As an example, Song *et al.*[51] made silicon carbide (SiC) QDs by a chemical etching technique that collective SiC nanoparticles (firstly generated by self-propagating combustion synthesis) were dissolved in a mixture of nitric and hydrofluoric acids. The incised substance was then sonicated followed with ultra-gravity chromatography to produce an aqueous solution of QDs. Similarly, Olaoye *et al.*[52] employed hydrothermal and wet etching of 3C-SiC to obtain SiC quantum dots. They demonstrated that the electrochemical energy gap between HOMO and the LUMO levels of 3C-SiC QDs was in close correspondence to the trend of optical bandgaps by cyclic voltammetry. In the analysis by transmission electron microscopy (TEM), it was also determined that the size of the particles reduced as the etching time increases. Unetched sample formed aggregated bulk crystals of approximately 19.06 nm, whereas etched colloidal suspensions obtained finally clear QD solutions with successively smaller average sizes of approximately 2.02 nm, 1.75 nm, 1.18 nm, and 1.15 nm after the 30 minute, 1 hour, 1.5 hour, and 2 hours of etching, respectively (Fig. 10(a)).[53]

While the top-down approach offers flexibility in nanostructured system design,[53] it suffers from structural defects arising from contaminant inclusion during processing.[54] The bottom-up method constructs materials at the atomic and molecular level and in particular, pathetic stages the clusters into QDs. This approach enables precise control over quantum confinement by building QDs from molecular precursors

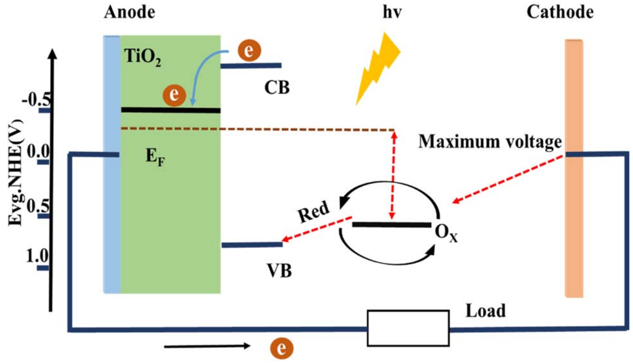


Fig. 8 Principle of operation and structure of a QDSSC.[5]

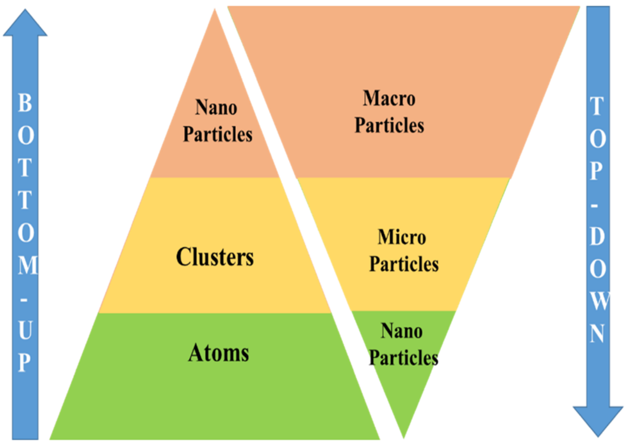


Fig. 9 Diagrammatic illustration of top-down and bottom-up methods for QD synthesis.[51]

through vapour-phase or solution-based methods.[55] There are two general nanofabrication approaches to bottom-up QD synthesis to which, wet chemistry and vapor-phase processes. Examples of well-known wet methods are hydrothermal synthesis, sol–gel, nano emulsion, stepwise organic, hot-injection decomposition, and microwave-assisted techniques whereas vapor-phase techniques are physical or chemical vapor deposition and epitaxial growth.[56] One popular technique for creating carbon quantum dots (CQDs) is the hydrothermal process.

2.3. Fabrication approaches for quantum dot-based solar cells

There are many sophisticated methods that are used in the ways of preparing QDs and QDSCs; they include self-assembly, electrical gating, chemical pyrolysis, colloidal synthesis, conventional aqueous methods, MOCVD, and molecular beam epitaxy (MBE).[57,58] The deposition of the QD layer depends on numerous spin-coating or dip-coating steps. The concentration of the QD employed, as well as spin or dip cycles, determines the QD thickness. The final solar cells made using both techniques operate quite similarly and are highly adjustable in terms of ligand exchange and layer thicknesses. Each of the two deposition methods possesses its advantages and disadvantages. Dip coating requires reasonable overall volume to totally cover the substrate. Thus, the concentration of the QD solution employed in the process of dip coating (*e.g.*, 1020 mg mL) is generally less than that of spin coating (30 mg mL). Dip coating allows for tighter control and can deposit more solar cells with a single QD synthesis because of the incredibly thin QD films that are formed per cycle. However, because only a limited quantity of QDs deposited each time, this deposition procedure often takes longer. This hyper steady deposition will necessitate a QD increased solution concentration producing an easier film construction and *vice versa* of finer layers.[59] Wang *et al.*[59] have used surface engineering to increase QD loading in QDSCs. Secondary deposition was made by depositing excess ZCISe (Zn–Cu–In–Se), ZCIS (Zn–Cu–In–S), or CdSe QDs onto previously sensitized TiO_2 films using ammonium cationic surfactants (Fig. 11).

Increment in QD loading increased short circuit current density (J_{sc}) and power conversion efficiency (PCE) and led to a higher solar harvesting. A record PCE of 10.26% in the QDSCs using Cu_2S/brass counter electrodes in simulated AM1.5G beam was recorded with this secondary deposition of ZCISe QDs.[60] Using Gao *et al.* as an example, they used a hydrothermal method to produce graphene quantum dots (GQDs) and used them as a part of c-Si/GQD heterojunction solar cells. This structure allows effective segregation of photogenerated electron–hole pairs at the interface to prevent charge recombination at the anode, and electrode to electron conversion in the GQDs is efficient. These effects aided in enhancing photovoltaic performance and stability of the device. The c-Si/GQD-based solar cells stored longer than six months of operation and had the maximum PCE of 6.63% (Fig. 12).[61]

2.4. Mathematical modelling and simulation of quantum dot-based solar cells

Mathematical modelling and simulation are essential tools in the development of third-generation QDSCs, enabling in-depth analysis of device physics, structural parameter optimization, and performance prediction prior to experimental fabrication. Before the experimental fabrication, researchers usually perform thorough preliminary evaluation with the help of advanced simulation tools to refine device architecture and predict the way it will operate. Solar cell modelling has been implemented across various software platforms including SILVACO Technology Computer-Aided Design (TCAD), Lumerical, COMSOL Multiphysics, and Solar Cell Capacitance Simulator in One Dimension (SCAPS-1D), each offering distinct capabilities for optical and electrical simulation. Simulation studies are also informative on the topic of recombination mechanism, determining its type and location anywhere in various device structures. Also, the concentration of dopant and the density of the traps in nanocrystal layers can be properly estimated. This ensures that blocking contacts are chosen well and optimized to enhance further photovoltaic performance. Density functional theory (DFT) calculations have further been employed to investigate the electronic structure of QD surface ligands and

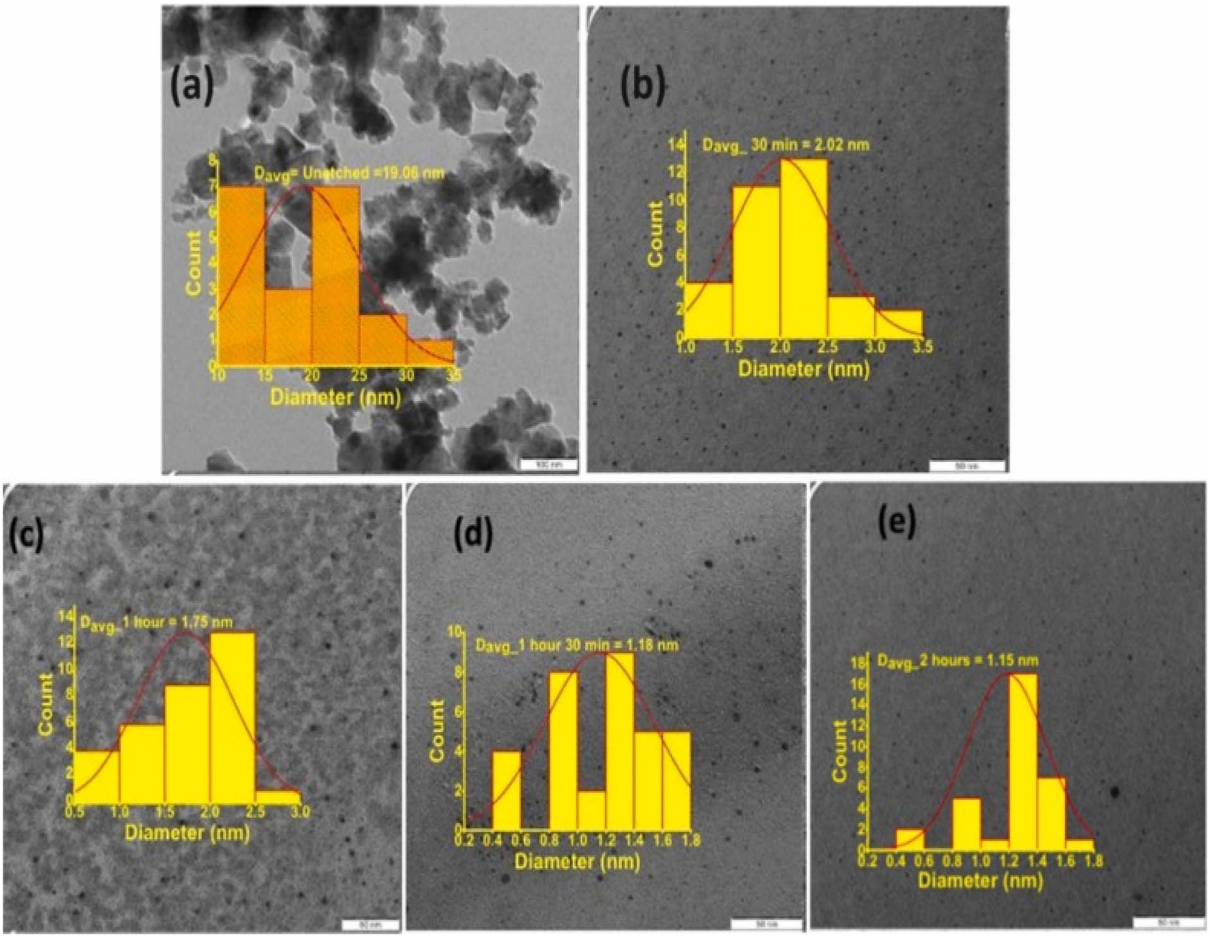


Fig. 10 TEM micrographs and corresponding particle size distribution histograms of 3C-SiC quantum dots obtained at different etching durations: (a) unetched sample, (b) 30 min, (c) 1 h, (d) 1 h 30 min, and (e) 2 h etching. The average particle diameters decreased from 19.06 nm for the unetched sample to 2.02, 1.75, 1.18, and 1.15 nm after progressive etching, respectively.[52]

predict optimal passivation strategies, while drift-diffusion models implemented in tools such as COMSOL and SCAPS-1D enable systematic evaluation of recombination pathways, trap densities, and contact selectivity across different QDSC architectures.[62–64] The SILVACO TCAD platform is very popular in the modeling of QDSC. In the example of Mehrabian *et al.* the simulation of an ITO/TiO_2/CdS/P_3HT/PCBM/Ag structure was done using this tool in which the bulk QDs layer was a densely packed sheet of QDs.[65,66] PbS QD nano cylinders were formed over a remaining PbS layer that was coated with ZnO in another set-up. In this design, the nanopatterning was limited to intrinsic n-junction with the front and back connection point and the p-type material being planar. The interposed additional layers of QD between the n-type ZnO and the Au back contact

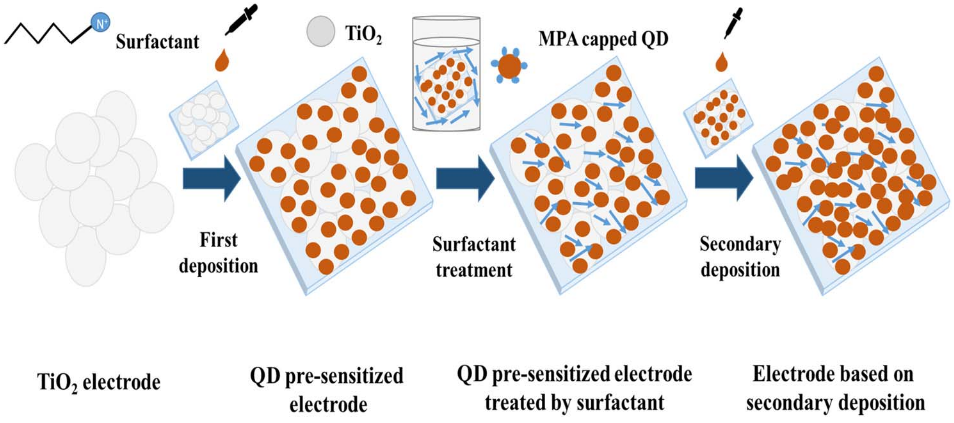


Fig. 11 Surface ligand assisted assembly technique for secondary deposition-based QD-sensitized photoanode synthesis.[5,60]

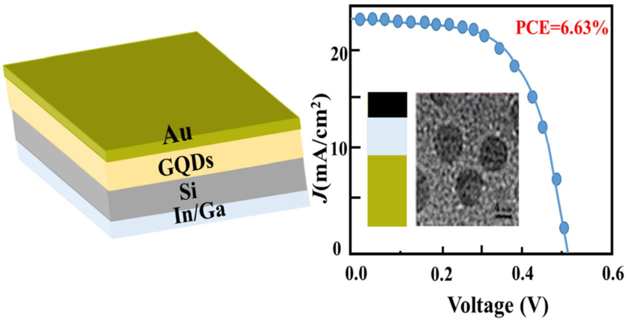


Fig. 12 (Left) Heterojunction solar cell based on c-Si/GQD. Parametric plot (sin(*x*), cos(*x*)) on the right.[61]

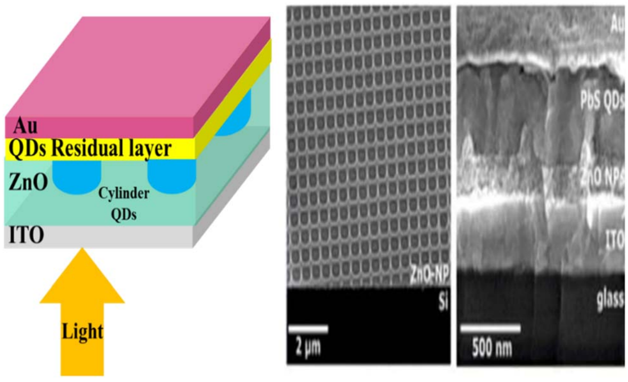


Fig. 13 (Left) A PbS quantum dot SCs patterned p–i–n heterojunction structure, with light originating from the bottom. ITO is the front contact, and Au is the back contact. ZnO is the n-type layer, and bulk PbS quantum dots are the p/i-type layer, which together create a three-dimensional interface. (Middle) SCIL-patterned ZnO nanoparticle layer on a silicon substrate seen from a SEM perspective (451). (Right) The patterned cell structure in a SEM cross-section.[5]

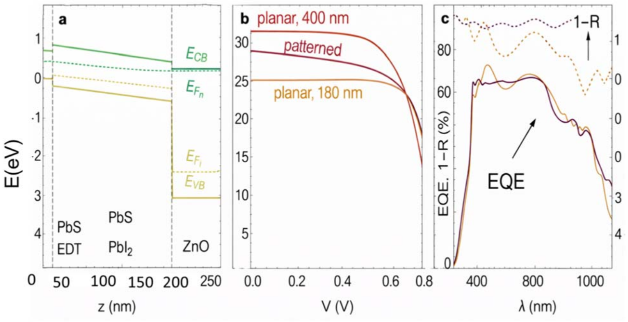


Fig. 14 (a) PbS quantum dot solar cell band diagram with an active layer of 180 nm under J_{sc} conditions ($V = 0$). From top to bottom, the valence band, electron quasi-Fermi level (E_{Fn}), hole quasi Fermi level (E_{Fp}), and conduction band are displayed. The various areas of the p–i–n junction are indicated by grey vertical dashed lines. The light comes from the right. (b) *J*–*V* characteristics were simulated for planar cells with absorber thicknesses of 180 nm (orange) and 400 nm (red) and a patterned absorber layer (purple). (c) The external quantum efficiency (EQE) and wavelength-dependent reflection losses of a synthetic planar (orange) and patterned (purple) PbS quantum dot SC. The EQE trends are represented by solid lines, and the EQE upper limits are represented by dashed lines.[5,66]

was used as an electrical barrier.[67] The series was made of thin p-type and intrinsic QD layers and the forthcoming dimensions and square mat of the pillars were maximized accordingly, to accommodate the plasmonic modes and robust localized optical resonances, overall raising the light capturing and performance of the device. The nanostructured geometry greatly reduces the carrier transport pathways especially those that are produced on the rear side of the device. This was done through nanopatterning of holes of a layer of ZnO nanoparticles (ZnO-NP) deposited on ITO and then filling them with quantum dots (QDs). Nanopatterning of the ZnO electron transport layer using substrate-conformal soft-imprint lithography (SCIL) was employed to enhance light trapping, with optical simulations confirming an improvement in absorption per unit volume by a factor of approximately 19.5.[68]

Having incorporated the QD pillars into the ZnO framework, Tabernig *et al.* scaled the dimensions of the structure to optimize the functioning of the device.[69] They used Lumerical software to perform finite-differentiation time-domain (FDTD) optical simulations and used the CHARGE solver to analyze charge transport by the drift diffusion model. The simulations looked at optical absorption in bulk regions of PbS QD to calculate the best absorption per unit area in the patterned absorber. In the AM1.5G solar spectrum, electronics properties such as recombination rates, doping density, charge hopping, and the voltage loss accompanying defect induced active conduction band states were systematically studied.[70]

Patterning has been shown to slightly enhance the open-circuit voltage and increase the current density by up to 3.2 mA cm^{-2}, leading to an overall improvement in device efficiency of approximately 0.4%. This enhanced the performance by transferring quantum dot (QD) nanopillars to a 70 nm-thick substrate of ZnO residual utilizing a square lattice structure with its pitch size set to 500 nm. Besides the improvement of the current generation, the patterned architecture is also found to adjust the distribution of electric field inside the absorber layer, which consequently has an impact on the fill factor (FF), as the simulation investigations confirmed. Patterned experiments found by Tabernig showed an increase in current density of 0.74 mA cm^{-2}, as shown on Fig. 13. This was improved with reference to the better infrared sensitivity just like the simulation results. Fig. 14(a) shows the electrical band diagram of a planar device having a 180 nm-thick absorber assuming that zero bias is applied on the *z*-direction. It is possible to distinguish three clear regions which are related to the p, i and n-type layers. A band bending process in depletion-type heterojunction solar cells takes place across an intrinsic (i-type) region creating a built-in electric field that assists in separating charge. Due to the variation in bulk QD energy, the p-type QD layer has a reduced energy offset than the i-type layer; to further study the electrical performance of patterned QDSCs, simulated patterns of current voltage (IV) characteristics of a planar and patterned QDSC with the absorber thickness of 180 nm and 400 nm, respectively, under AM1.5G illumination are given in Fig. 14(b). The improvement of light trapping in the patterned structure

Table 2 Comparative overview of quantum dot absorber materials used in QDSCs

Material system	Bandgap (eV)	Representative reported PCE (%)	Toxicity	Stability	Key advantage	Major limitation	Optimal architecture	References
PbS QDs	0.4–1.5	11.3	High (Pb)	Moderate	Broad NIR absorption; size-tunable bandgap	Lead toxicity; oxidation instability	Depleted heterojunction/hybrid	71 and 72
CdSe QDs	1.7–2.7	Moderate efficiencies reported	High (Cd)	Moderate	High absorption coefficient; MEG potential; visible-light tunability	Cd toxicity; limited NIR absorption	Sensitized QDSSC/ CdS–CdSe bilayer	73
Sn:InP QDs	~1.3	3.54	Low (Pb-free)	Good	Environmentally benign; improved band alignment *via* Sn doping	Complex synthesis; lower efficiency	Sensitized QDSSC (TiO_2 scaffold)	72 and 74
Perovskite QDs	1.5–2.3	18.3 (certified)	High (Pb)	Low (moisture/ thermal sensitivity)	Highest PCE; defect tolerance; long carrier diffusion	Moisture and thermal instability; Pb toxicity	Hybrid/tandem (perovskite-Si)	17
Carbon QDs (CQDs)	~2.2–3.0	Moderate efficiencies reported	Very low	Excellent	Non-toxic; low-cost synthesis; photostable	Low charge mobility; limited NIR harvesting	Flexible QDSSC/ Co-sensitizer	75 and 76
$CuInS_2$ QDs	1.5–1.8	~4–7	Low	Moderate	Cd/Pb-free; broad absorption; cost-effective	Carrier transport limitations; stability concerns	Sensitized QDSSC/ liquid-junction	19 and 77

can be validated by the increase of short-circuit current density (J_{sc}) and the improvement of the external quantum efficiency (EQE) as indicated in Fig. 14(c). Though by slightly lowering the FF values, the experiment allows less efficient carrier extraction in the patterned format, the open-circuit voltage (V_{oc}) is not influenced, and it suggests that the enhanced surface area does not induce any important new recombination losses.

3. Advances in material preparation for QDSCs

The choice of materials and its engineering is crucial when it comes to efficiency, stability and scalability of QDSCs. An average QDSC system has multi-layers functionalities, which are the quantum dot absorber, electron transport material (ETM), hole transport material (HTM), and electrodes. The components play different roles in terms of light absorption, charge separation, transport and collection.

3.1. Classification and comparison of QDSCs based on materials used

In order to assess the recent developments in a systematic fashion, the materials employed in QDSCs can be broken into four key groups, which are summarized in Tables 1–4.

Notably, CQD-based co-sensitized DSSCs have achieved power conversion efficiencies of up to ~9% when integrated with N719 dye sensitizers, whereas standalone CQD sensitizers generally exhibit comparatively lower photovoltaic performance due to limited charge transport and narrower spectral utilization. QDSCs employ certain materials to improve light absorption as well as charge transport and device longevity. Table 2 displays the components.[72] QDSCs are the subject of most research because of their ability to absorb visible and infrared light with depending on stability traits. After capping with oleic acid, QD cell performance is constant due to a decrease in inter dot coupling. When compared to unmodified TiO_2, the nontoxic doping approach with Sn increases the efficiency by 35% by providing TiO_2 scaffolds with improved charge injection.[72] Table 2 presents a comparative overview of various quantum dot material systems employed in QDSCs. PbS and perovskite quantum dots exhibit superior photovoltaic performance due to their tunable bandgaps and enhanced light-harvesting capability. However, toxicity and long-term stability remain major concerns for these materials. In contrast, carbon and InP-based quantum dots provide environmentally friendly alternatives, although their efficiencies are comparatively lower. Therefore, the selection of quantum dot materials depends on the targeted photovoltaic application, efficiency requirements, environmental considerations, and device stability.

As illustrated in Table 3, the selection of electron and hole transport materials critically governs charge extraction efficiency, interfacial recombination losses, and overall device stability in QDSCs. Among electron transport materials, mesoporous TiO_2 remains the most widely employed ETM owing to its chemical stability, appropriate conduction band alignment, and compatibility with a broad range of QD sensitizers;

Table 3 Comparative overview of electron and hole transport materials used in QDSCs

Layer type	Material	Mobility ($cm^2 V^{-1} s^{-1}$)	Best PCE achieved (%)	Advantages	Disadvantages	References
(A) Electron transport materials (ETMs)						
ETM	TiO_2 (mesoporous)	0.1–4	Baseline (widely used)	Stable; ideal band alignment; mature technology	Low electron mobility; slow electron transport	74
ETM	ZnO	200–300	18.24% (TiO_2/ZnO hybrid)	High electron mobility; transparent; fast charge extraction	Interfacial instability; reacts with perovskite	78
ETM	TiO_2/ZnO hybrid	—	18.24%	Combines TiO_2 stability with ZnO mobility; improved band alignment	Complex dual-layer deposition; optimization required	74 and 79
(B) Hole transport materials (HTMs)						
HTM	Spiro-OMeTAD	2×10^{-4}	23.14% (V_{oc} enhancement)	Favorable HOMO alignment with QDs; widely validated	Hygroscopic; requires dopants; expensive	80
HTM	Graphene oxide (GO)	—	13.84%	Accelerates hole transfer; suppresses recombination; flexible	Electrical properties depend on oxidation degree	81
HTM	PEDOT:PSS	10^{-3} to 10^{-2}	2.79%	Low-cost; flexible; solution-processable	Acidic nature may degrade QDs; relatively low hole mobility	82
HTM/counter electrode	Cu_2S	—	4.06%	High catalytic activity; efficient hole extraction; inorganic stability	Limited application in solid-state devices	83

however, its relatively low electron mobility of 0.1–4 $cm^2 V^{-1} s^{-1}$ limits charge extraction rates under high illumination conditions. ZnO offers a substantially higher electron mobility of 200–300 $cm^2 V^{-1} s^{-1}$, enabling faster charge extraction and reduced recombination losses, yet its interfacial instability and tendency to react with perovskite materials at elevated temperatures remain significant concerns. The hybrid TiO_2/ZnO electron transport layer effectively combines the chemical stability of TiO_2 with the superior charge transport properties of ZnO, achieving a power conversion efficiency of 18.24% the highest reported among ETM configurations evaluated in this review demonstrating that composite ETM architectures represent a particularly promising direction for high-performance QDSC development.[74] Among hole transport materials, spiro-OMeTAD demonstrates the most favorable HOMO level alignment with QD absorber layers, facilitating efficient hole extraction and contributing to open-circuit voltage enhancements reaching 23.14%; however, its hygroscopic nature, requirement for chemical dopants, and high material cost limit its applicability in large-scale and flexible device formats. Graphene oxide represents a compelling alternative, offering accelerated hole transfer kinetics and suppressed charge recombination while maintaining mechanical flexibility, though its performance remains sensitive to the degree of oxidation.[80] PEDOT:PSS offers the lowest fabrication cost and excellent solution-processability suited to flexible substrates, but its acidic nature can degrade certain QD materials at the HTM/QD interface, limiting its compatibility with moisture-sensitive systems. Cu_2S functions effectively as both an HTM and counter electrode in polysulfide-based QDSSCs, combining high catalytic activity with efficient hole extraction, though its application in solid-state device architectures remains limited. Overall, the choice of HTM must be carefully matched to the QD absorber system, device architecture, and target application to minimize interfacial energy losses and maximize operational stability.

The research indicates that the hybrid TiO_2/ZnO mesoporous structure improves band matching between perovskite layers, leading to increased electron injection rates, as Table 3 illustrates. TiO_2 is the most commonly used ETM because it is competitively stable and has appropriate band alignment. ZnO has a better electron mobility, but it is interfacially unstable. Bilayer and SnO_2 based ETMs are the new developments that predominantly focus on the effectiveness of charge extraction and stability of the devices.[80]

The hole transport materials (HTMs) have the job of removing holes out of the QD absorber with minimal interfacial energy loss and recombination. Open-circuit voltage and stability of operation is strongly dependent on the choice of HTMs. Table 3 also indicates a representative HTM in QDSCs. Spiro-OMeTAD high HOMO level (−5.0 eV) effectively extracts holes by matching perovskite valence bands. As shown in Table 3,[84,85] graphene oxide improves photocurrent efficiency by decreasing charge recombination between QDs and connections between electrolytes. The elements, supplies, and features for charge collecting are shown in Table 4 as well as structural soundness.

Table 4 Electrodes and counter electrodes used in QDSCs

Component type	Material	Role	Advantages	Limitations	References
(A) Transparent front electrodes (anodes)					
Transparent anode	ITO	Primary transparent conducting electrode; electron collection and transport	High transparency (>85%); low sheet resistance; mature technology	Brittle; indium scarcity; costly sputtering	86
Transparent anode	FTO	Thermally stable transparent electrode; preferred for sintered TiO_2 photoanodes	High thermal/chemical stability; polysulfide-resistant; cost-effective	Lower conductivity than ITO; surface roughness increases recombination	87
Transparent anode	Ag nanowire (AgNW)	Flexible transparent electrode for roll-to-roll QDSC fabrication	Flexible; solution-processable; tunable sheet resistance	Ag oxidation; junction resistance; limited stability	88
(B) Metal back contacts (cathodes)					
Metal cathode	Gold (Au)	High work-function back contact; hole collection in p-type QD layers	Excellent conductivity; chemically inert; efficient ohmic contact	Very high cost; Au diffusion at high temperature	89
Metal cathode	Aluminium (Al)	Low work-function cathode for n-type extraction and Schottky junctions	Low cost; lightweight; simple thermal evaporation	Easily oxidized; poor p-type QD compatibility	90
Metal cathode	Silver (Ag)	Conductive back contact for perovskite and hybrid QDSCs	High conductivity; lower cost than Au; reflective for light trapping	Sulfidation; requires interfacial buffer layer	91
(C) Counter electrodes (for QDSSCs)					
Counter electrode	Cu_2S/brass	Electrocatalytic CE for polysulfide redox (S^{2-}/Sn^{2-}) reactions	High catalytic activity; low charge-transfer resistance; inexpensive	Brass corrosion; limited long-term stability	92
Counter electrode	C-Fabric/WO_{3-x}	Composite CE: WO_{3-x} for catalysis; C-fabric for conductivity and flexibility	Synergistic activity; flexible; good chemical stability	Complex fabrication; lower conductivity than Cu_2S	93
Counter electrode	Platinum (Pt)	Catalytic CE for I^-/I_3^- redox in iodolyte-based QDSSCs	Excellent catalytic activity; stable; low charge-transfer resistance	Expensive; poisoned by polysulfide electrolyte	94
Counter electrode	Carbon black/ Graphene	Low-cost CE for polysulfide systems; graphene enhances conductivity	Earth-abundant; low cost; polysulfide-compatible	Lower catalytic activity than Cu_2S; high sheet resistance	95

As summarized in Table 4, electrode selection critically influences both the optical and electrical performance of QDSCs. Among transparent front electrodes, ITO and FTO remain the industry standard due to their well-established optical transparency exceeding 85% and low sheet resistance; however, the brittleness of ITO and its dependence on scarce indium resources motivate the development of flexible alternatives such as silver nanowire networks, which offer comparable transparency with solution-processable deposition compatible with roll-to-roll manufacturing.[86,87] For metal back contacts, gold remains the benchmark due to its high work function and chemical inertness, enabling efficient ohmic contact formation in PbS depleted heterojunction devices; nevertheless, its prohibitive cost and tendency to diffuse into QD layers at elevated temperatures limit its scalability, driving interest in silver as a cost-effective alternative when appropriate interfacial buffer layers are employed.

Among counter electrode materials, Cu_2S on brass substrates remains the most widely adopted choice for polysulfide-based QDSSCs owing to its high electrocatalytic activity and low charge-transfer resistance, though brass corrosion under prolonged polysulfide exposure presents a long-term stability challenge. Platinum, while exceptionally effective for iodide/triiodide redox systems, is severely poisoned by polysulfide electrolytes and is prohibitively expensive for large-scale deployment. Carbon-based counter electrodes, including carbon black and graphene composites, represent the most promising low-cost alternative, offering earth-abundant composition and polysulfide compatibility, with graphene variants providing enhanced conductivity and electrocatalytic

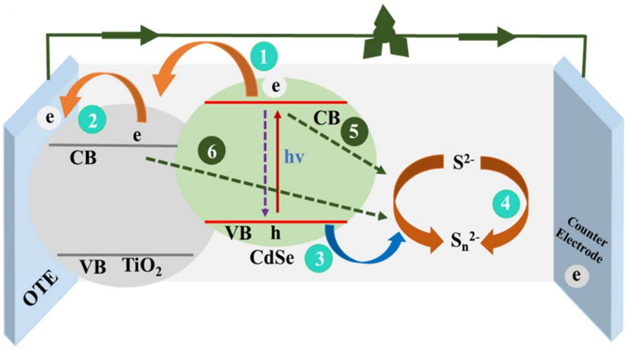
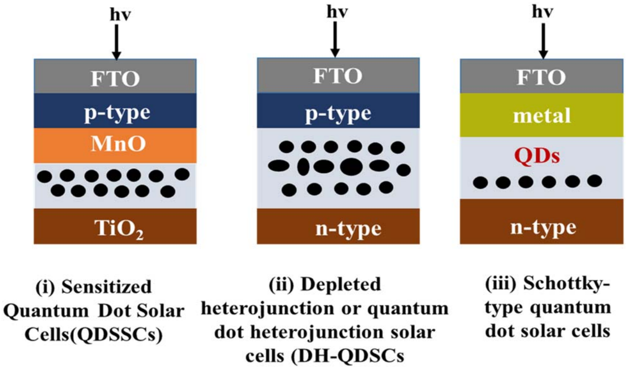


Fig. 15 Diagrammatic representation of photo induced charge-transfer processes after a laser pulse excitation.[11]



(i) Sensitized Quantum Dot Solar Cells(QDSSCs)

(ii) Depleted heterojunction or quantum dot heterojunction solar cells (DH-QDSCs)

(iii) Schottky-type quantum dot solar cells

Fig. 16 The three main QDSCS architectures.[51]

surface area. The composite C-fabric/WO_{3-x} architecture further demonstrates that synergistic combinations of catalytic and conductive components can simultaneously address the conductivity and activity limitations of single-material counter electrodes, setting a direction for future scalable QDSC manufacturing.[93]

Combining carbon fabric with WO_{3-x} counter electrodes results in strong catalytic activity from WO_{3-x} and low sheet resistance from C-fabric, setting new performance records. A 15% increase in V_{oc} results from improved hole extraction in PbS QDSCs caused by the application of PDTPBT polymers on ITO anodes.[95] The conversion of oleic acid to MPA during ligand exchange affects both the stability of the device's operation and the performance of the inter-diet coupling. Fluorinated graphene is added to spiro-OMeTAD to increase its high-temperature stability. Environmentally friendly QD materials like InP and hybrid architectures are used in materials development research to push QDSC efficiency values near its theoretical 66% limit.[84] The schematic representation of photo induced charge-transfer processes after a laser pulse excitation is shown in Fig. 15.

4. Principal architecture of quantum dots solar cells

It is necessary to examine the three main architectures of QDSCs (i) sensitized QDSSCs, (ii) depleted heterojunction or quantum dot heterojunction solar cells (DH-QDSCs), and (iii) Schottky-type QDSCs in order to comprehend their structural arrangement, operating principles, and charge transport layers. We can have a better grasp of the physical organization of the active layers as well as the mechanisms underpinning charge generation, separation, and collecting by comprehending these structures.

4.1. Sensitized quantum dots solar cells

The QDSSC is the most researched of the various QDSC architectures. Its working principle is quite similar to that of dye-sensitized solar cells (DSSCs) the main difference is that instead of organic dye molecules, QDs are used to sensitize the cell. When using the standard QDSSC setting, a wide-bandgap semiconductor oxide (TiO_2, ZnO, or SnO_2) is applied on the photoanode and coated with QDs.[96,97] Whenever the QDs receive incident photons, they create photo excited electrons which are injected into the conduction band of the semiconductor oxide. After injection, electrons are carried through the TiO_2 network by fast diffusion channels, and charge compensation is done over the liquid electrolyte by diffusion limited redox reaction, typically between pair of couples (*i.e.*, I_1-/I_3- or S_2-/Sn_2-).[98] The redox electrolyte then deoxidizes QDs and the counter electrode promotes the reduction of the oxidized species completing the circuit (Fig. 16).

Even though size-tunable absorption offers benefits and multiple exciton generation can be achieved, the efficiency of QDSSCs is still low. The causes of performance losses are charge recombination along the QD/electrolyte interface, inadequate QD loading or surface coverage, low carrier diffusion lengths, chemical instability and corrosion of QD sensitizers, and loss of electrolyte, and degradation of QDs.[86] Specifically, charge recombination at the TiO_2 electrolyte/electrode interface plays a potent role in the influence of open-circuit voltage (V_{oc}) on the performance of the device, which poses a significant limitation in the device and is a significant aspect of constraint. Table 5 is a comparative analysis of DSSCs and QDSSCs.

4.2. Quantum dots heterojunctions solar cells

The DH-QDSC takes the similar device structure of the traditional thin-film solar cells. This architecture was invented to overcome the interfacial recombination losses and stability problems that are usually related to liquid electrolyte-based systems. Unlike the QDSSCs, where the QDs are used as sensitizers, DH-QDSCs uses light absorption based on a p–n or n–n heterojunction. QDs with different n-type material, including TiO_2, ZnO, or SnO_2 are simply deposited on other parts in this design, such as PbS, PbSe, or CdTe. This heterointerface is formed and creates a depletion region which helps ease the separation of charges during illumination. Structurally, the layer of QD absorber is between the n-type ETL and the p-type hole transport layer (HTL). Exciton dissociation thus takes place at the depletion region and the ETL/QD and HTL/QD interfaces as well.[102] DH-QDSSC architecture has higher carrier collection efficiency and device stability in comparison to liquid junction QDSSCs. Still, there are still some difficulties,

Table 5 Comparison of QDSSCs and DSSCs

Feature	QDSSCs	DSSCs (dye-sensitized)	References
Light absorber	Quantum dots (tunable bandgap)	Organic dyes (fixed bandgap)	99 and 100
Efficiency	Up to 13.4%	∼12%	36
MEG utilization	Yes (enhanced photocurrent)	No	101 and 102

especially the reduction of interfacial defects and the uniformity of the electron and hole transport that are essential to the optimization of future performance.[103]

4.3. Schottky-type quantum dots solar cells

QDSCs of Schottky type are based on a metal–semiconductor junction to provide charge separation. This layout, the carriers (pores) generated during photogeneration are easily separated without an extra layer of hole transporter, or liquid electrolyte and so makes this structure of a device simpler. Normally, a film of QD is directly deposited on a metallic surface (*i.e.* Au, Ag, or Al) creating a Schottky junction on the interface as the material binds. The metal to semiconductor interface has an inherent electric field which under illumination causes the delocation of electrons and holes.[104] After photo exciting the QD layer, the holes flow into the QD layer to the back contact, and the electrons flow out of the metal electrode. The simplicity of structure and simple fabrication of the Schottky-type QDSCs have drawn a lot of research. Furthermore, their speed in response to photo sensation qualifies them to be utilized to integrate plasmonic metals to improve the light trapping and optical absorption to create some properties.[105] Irrespective of these benefits, in comparison to heterojunction-based devices, they generally have lower power conversion efficiencies. This is due to relatively poor separation of carriers, recombination loss, and low open-circuit voltage (V_{oc}) due to pinning of Fermi-level at the interface between the metal and semiconductor.[106] To conclude, three major QDSC designs, namely, Schottky-type QDSCs, DH-QDSCs, and QDSSCs, are extensively studied (Fig. 16). The configurations have different charge generation mechanisms and transport mechanisms, which are one of the chief factors that limit their performance capabilities. The band alignment and the process of photogeneration carrier transport in the QDSCs are schematically represented by Fig. 17.

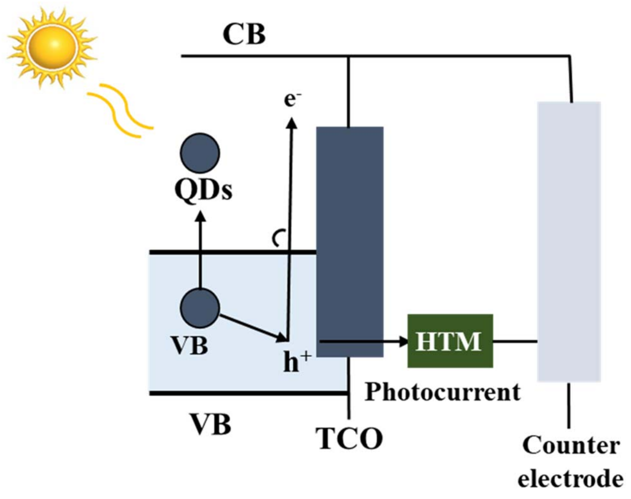


Fig. 17 Band structure and photogenerated charge flow schematic representation in QDSCs.[51]

4.4. A brief comparison of architectures

The architecture of QDSC has been observed to possess unique operational mechanisms, efficiencies and technological challenges with respect to the structural configuration. Schottky junction QDSCs are the simplest device structure of the group of the QDs, in which the QDs are in direct contact with a metal electrode. The built-in electric field at the metallic-QD interface is used to separate the charges but the carrier mobility and recombination losses also limit the power conversion efficiency (PCE) to 5 to 8 percent.[11,107] By contrast, QDSSCs use a wide-bandgap mesoporous semiconductor backbone (*e.g.*, TiO_2 or ZnO) to immobilize QD sensitizers and electronically withdraw electrons effectively. The broad-spectrum absorption of QDs generated by the tunable bandgap along with the potential to generate multiple exciton (MEG) makes the efficiencies of QDs to be up to ∼13.4. However, it has the disadvantage of allowing long term stability issues and interfacial recombination losses with the use of liquid electrolytes/polysulfide.[107,108]

Bulk heterojunction QDSCs consist of quantum dots of conductive polymer and an interpenetrating network of donors and acceptors to dissociate exciton and allows low temperature processing in solution. Performances of these devices are usually within the range of 6–10 percent yet its performances heavily rely on morphology control and phase segregation of the QDs and polymer matrices at nanoscales.[109] To leverage the complementary optical and electronic characteristics of QDs and conventional photovoltaic platforms, *e.g.* silicon or perovskite solar cells, hybrid QDSC architectures utilize the QDs on these platforms. In this type of structure, the light is able to be efficiently absorbed by the QDs and converting it into carriers; the design can also be as a spectral converter or serving as sensitizing layers. Hybrid devices have shown the most claimed efficiencies (maximum of about 18.1% or more in optimized systems), but interfacial engineering and material compatibility has been another huge hurdle.[110,111]

Generally, the most common architecture is the QDSSCs because of their compromise between adjustable absorption and the ease at which the device is fabricated, though hybrid QDSCs are currently being the most prospective in regard to high efficiencies obtained in terms of synergistic combination with established photovoltaic technologies. Generally, QDSSCs are the most extensively investigated architecture but because of

Table 6 Horizontal comparison of QDSC device architectures: efficiency, strengths, and applicability

Architecture	PCE range (%)	Fabrication complexity	Key strengths	Major challenges	Best-suited materials	Scalability	References
Schottky junction	5–8	Low	Simple fabrication; fast photoresponse; compatible with plasmonic enhancement	Low V_{oc} due to fermi-level pinning; high recombination at metal/QD interface	PbS, PbSe	High	107
Sensitized QDSSC	8–13.4	Moderate	Tunable absorption; MEG potential; mature TiO_2 scaffold technology	Electrolyte instability; interfacial recombination at QD/electrolyte interface	CdSe, $CuInS_2$, CQDs, Sn:InP	Moderate	108
Depleted heterojunction (DH-QDSC)	8–12	Moderate-high	Solid-state; no liquid electrolyte; better stability than QDSSC	Interfacial defects; precise band alignment required; complex deposition	PbS, PbSe, CdTe	Moderate	107 and 108
Bulk heterojunction (BHJ)	6–10	Moderate	Solution-processable; low-temperature fabrication; interpenetrating donor–acceptor network	Morphology control critical; phase segregation issues at nanoscale	QD-polymer composites (PbS/P3HT)	High	109
Hybrid/Tandem QDSC	Up to 18.3	High	Highest reported PCE; synergistic integration with Si/perovskite platforms; broad spectral coverage	Interface engineering complexity; material compatibility; high fabrication cost	Perovskite QDs + Si or perovskite thin-film	Low (current)	110 and 111

their trade-off between tunable absorption and device simplicity, hybrid QDSCs now offers the highest probability of reaching high efficiencies by using synergistic integration of the incorporation into mature photovoltaic technologies.

As evident from Table 6, each QDSC architecture presents a distinct trade-off between efficiency, fabrication complexity, and scalability. Schottky junction devices offer the simplest fabrication route and highest scalability potential, making them attractive for low-cost applications, yet their inherently low open-circuit voltage due to Fermi-level pinning at the metal/QD interface fundamentally limits their PCE to the 5–8% range. Sensitized QDSSCs currently represent the most extensively investigated architecture, benefiting from the mature TiO_2 mesoporous scaffold technology and the potential for multiple exciton generation (MEG); however, long-term electrolyte instability and interfacial recombination remain critical barriers to commercial deployment. Depleted heterojunction QDSCs offer a compelling middle ground eliminating the liquid electrolyte while maintaining solid-state charge transport though achieving defect-free interfaces with precise band alignment continues to challenge researchers.

Among the architectures evaluated, hybrid and tandem QDSCs currently lead in power conversion efficiency, with certified PCEs reaching up to 18.3% through synergistic integration of perovskite QDs with silicon or perovskite thin-film platforms. However, their high fabrication complexity and currently limited scalability represent significant obstacles to commercialization. Bulk heterojunction devices, while offering solution-processability and low-temperature fabrication advantages, require precise morphology control at the nanoscale that remains technically demanding. Overall, the selection of QDSC architecture should be guided by the intended application Schottky and BHJ architectures are better suited for flexible and large-area applications where cost and scalability are prioritized, while hybrid tandem configurations are more appropriate for high-efficiency stationary photovoltaic systems where fabrication cost is secondary to performance. Future progress will likely depend on combining the scalability advantages of sensitized QDSSCs with the stability benefits of solid-state heterojunction designs through innovative interface engineering approaches.

Among these, hybrid architectures currently demonstrate the highest reported efficiencies due to the combination of QD spectral engineering and mature photovoltaic platforms. QDSSCs offer strong theoretical advantages through MEG; however, long-term stability and scalability remain limiting factors.

5. Performance and efficiency of QDSCs

Since QDSCs are an alternative to silicon-based solar cells, they represent a viable third-generation photovoltaic technology. Because of their special quantum confinement characteristics, quantum dots serve as the primary light-absorbing component in QDSCs. Three characteristics set the light-absorbing quantum dots apart: their ability to produce numerous excitons, their bandgap tunability, and their high extinction coefficient.[45] The choice of materials, surface passivation techniques, and device structural design are the three main factors that affect QDSC performance and efficiency. In the past, labs have studied QD solutions free of hazardous heavy metals including Pb and Cd. By applying efficient surface passivation methods to CIS QDs, high-photovoltaic-quality CIS/ZnS core/shell structures are created, increasing the efficiency of solar cells. Due to their perovskite characteristics and great efficiency, all inorganic $CsPbI_3$ perovskite QDs have attracted a lot of research attention. Higher levels of photovoltaic performance can be achieved by surface stress engineering $CsPbI_3$ PQDs to improve phase stability and optoelectronic properties. The main material option for QDSC devices is PbS QDs. Compared to standard ligand passivation techniques, surface passivation using triple-cation perovskites yields better photovoltaic results. Using iodide/triiodide and polysulphide electrolytes, Ag-doped CdS QDs produced by SILAR have demonstrated promise in solar cells. The presence of both surface defects and ligand molecules is crucial for QD performance. Surface engineering improves the performance of $CsPbX_3$ QDs and causes significant changes in optoelectronic behaviour.[112] Onium cations can be added to surface lattice regularizations that improve stability to address surface stress problems. Because of their enhanced Auger recombination, type II QDs provide QDSCs with higher V_{oc} and greater efficiency.

When there are resonances in the FP intensity peaks between the QD layers, backside mirrors and thin-film QDSCs function more effectively together, improving near-infrared photon absorption.[113] Core shell nanowire array designs composed of perovskite materials and QDs improve solar cell performance by enabling extended light absorption across the spectrum. The functionality of QDSSCs is significantly enhanced by the creation of electrodes with three-dimensional nanostructured properties. Currently, researchers focus on various approaches to improve QDSCs. Alkyl ammonium iodides have been used in ligand exchange strategies to improve the performance of organic-cation perovskite QD solar cells.[114]

When perovskite materials are used to passivate PbS QDs, both stability and efficiency are increased. By improving crystallinity and reducing defects, the use of hydroiodic acid (HI) in the synthesis of $CsPbI_3$ perovskite QDs increases the photoluminescence quantum yield and raises solar cell efficiency levels. The efficiency of QDSSCs has increased to over 15% in recent years as a result of increased focus on electron transport, surface chemistry, and quantum confinement research.[115] Although QDSCs continue to advance, they nevertheless confront current challenges. Although QDSCs have theoretical power conversion efficiencies of up to 66%, their real maximum efficiency is still below this threshold. This current gap has to be filled by future research. As of 2025, the performance level of QDSCs is 18.3%.[14] Researchers are still working to determine how stable perovskite solar cells, including those based on QDs, may be. Combining techniques like capping layers and size control adjustments is necessary to increase the moisture and heat resistance of perovskite solar cells. Because lead-based and cadmium-based QDs are environmentally hazardous, their combination causes problems for the environment. Research and development are currently underway for sustainable alternative QDs.[116] Because these advancements reduce flaws and enhance charge transport mechanisms, researchers should focus on surface passivation and ligand exchange strategies.[102] Researchers investigate novel QD material compositions to improve the processes of light absorption and charge production.[117] When utilized as parts of tandem solar cells, QD materials complement silicon and perovskite photovoltaic technologies, resulting in increased overall efficiency and a wider absorption range.[118] To improve device designs, researchers must investigate QD optoelectronic behaviour in

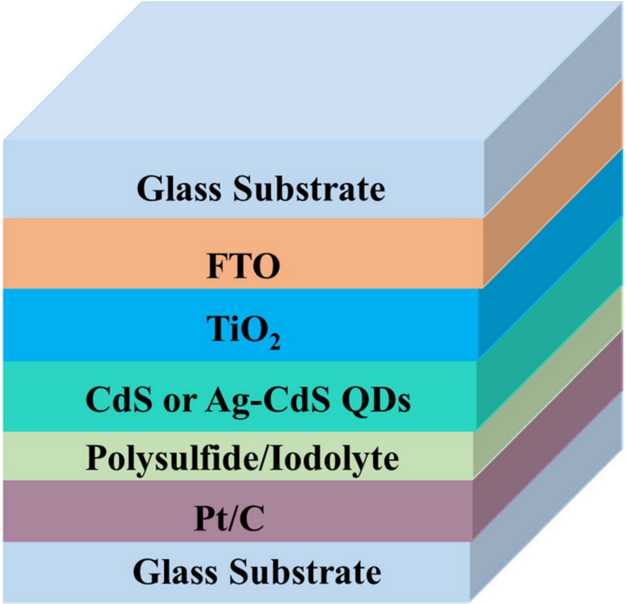


Fig. 18 An active thin-film technology, such as quantum dot solar cells or thin-film electronics, is represented by a multilayer device structure from cross-section.[20]

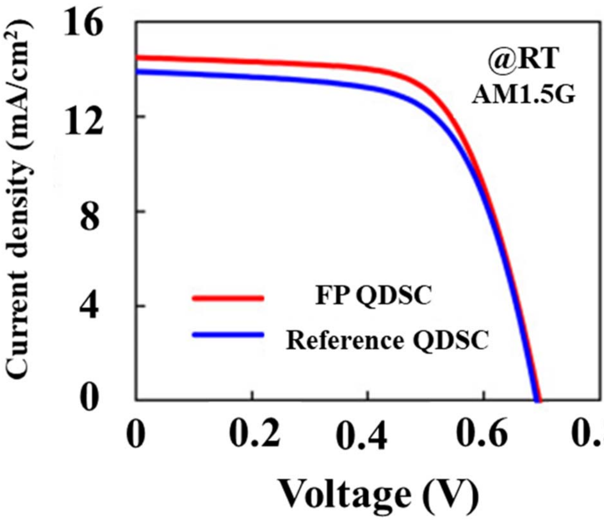


Fig. 19 Under AM1.5G illumination, the current–voltage (*I*–*V*) characteristic curve graph contrasts "FP QDSC" with "reference QDSC".[120,121]

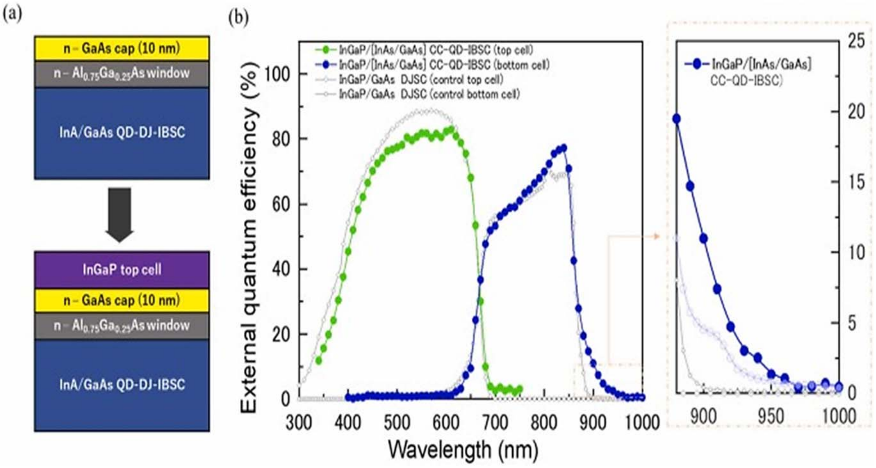


Fig. 20 Provides comprehensive details on the construction of quantum-dot-based photovoltaic cells together with a thorough examination of their functional characteristics in comparison to control cells. This analysis assesses the wavelength-dependent efficiency of QD-based devices and demonstrates their enhanced EQE performance.[29]

solar cell applications.[119] Fig. 18 shows how QDSCs overcome present obstacles and follow certain research paths to realize their potential as a low-cost, high-efficiency renewable energy source.

The sequential deposition of the glass substrate, FTO, TiO_2, CdS or Ag–CdS QDs, polysulfide/iodolyte electrolyte, and Pt/C counter electrode is depicted in Fig. 5 to illustrate how the device layers work together.[20] By displaying the impacts of light trapping on device performance, Fig. 19 provides a graphical representation of the electrical behaviour of the generated QDSCs.[120]

Fig. 20 shows how quantum dot solar cells overcome present obstacles and follow certain research paths to realize their potential as a low-cost, high-efficiency renewable energy source.

6. Efficiency enhancements in QDSCs

Increasing the efficiency rates of QDSCs is crucial for their effective future use. QD loading optimization, plasmonic improvements, ligand engineering, MEG, and hot carrier effects all contribute to an increase in PCE. The more QDs deposited on the photoanode structure, the more efficient light is absorbed and charge is generated. Secondary deposition and capping ligand-induced self-assembly (CLIS), two techniques for increasing loading efficiency, have shown promise.[122] It was demonstrated that the combination of ZCISSe quantum dot (QD)-sensitized TiO_2 with black phosphorus QDs results in a significant enhancement of the power conversion efficiency (PCE).[31] This is credited to the increase in light harvesting and effective transfer of charges between the sensitizer layer and transport layer.

Light absorption has also been enhanced to 11.0 percent in PbS based-QDSCs with the introduction of V-groove structures or compound parabolic trappers (VCPTs) which lower the escape probability of photons and improve optical confinement within the device.[123] Although these types of light-trapping strategies are often implemented in most photovoltaic technology types, there is always everyone who can further improve the absorption by introducing metal nanoparticles, say Ag or Au, by placing this close the QD layer. These metal nanostructures enhance optical performance through the effect of surface plasmon resonance (SPR) that enhances the local electromagnetic field and enhances greater absorption of photons in the active layer. When researchers use MPA instead of native ligands, device performance increases. Swapping out oleic acid since this modification improves the charge transfer of QD-photoanodes. After passivation, surface imperfections become less noticeable, boosting the stability of QD surfaces and decreasing non-radiative recombination, which boosts efficiency. Because quantum dots can create many excitons from a single photon, photocurrent levels can exceed the Shockley–Queisser limits.[124]

It is still challenging to handle this issue effectively. In order to increase voltage output, hot carriers in QDSCs must preserve energy prior to thermalization; yet, practical implementation is still challenging. Implementing large-scale manufacturing methods that maintain high efficiency and achieving environmental lifespan for QDSCs are crucial obstacles to solve. Improving QD-transport layer interfaces is still essential for reducing recombination and increasing the efficiency of charge transport.[125] The combined use of quantum dot properties to overcome technological challenges has the potential to transform QDSCs into a highly effective photovoltaic system that surpasses accepted limits.

As evident from Table 7, surface passivation through ligand exchange and secondary QD deposition represent the most practically accessible optimization strategies, delivering measurable PCE improvements while remaining compatible with existing colloidal synthesis and QDSSC fabrication platforms. Surface passivation has enabled PbS-based devices to reach 11.3% PCE with operational stability exceeding 1200 hours, while secondary deposition and capping ligand-induced self-assembly (CLIS) have pushed ZCISSe QDSC efficiencies from 13.54% to 15.31% through enhanced QD loading on TiO_2

Table 7 Horizontal comparison of key pptimization strategies for QDSC performance enhancement

Optimization strategy	Primary mechanism	PCE improvement	Advantages	Limitations	References
Surface passivation (ligand exchange)	Reduces trap-state density and suppresses non-radiative recombination	Up to 11.3% PCE (PbS with perovskite shell); stability retained for >1200 h	Simple and compatible with colloidal synthesis; improves both V_{oc} and J_{SC}	Ligand selection critically affects inter-dot coupling; organic ligands are prone to oxidation	17
Core–shell engineering	Shell passivates surface, confines carriers, and reduces Auger recombination	Enhanced quantum yield and improved operational stability; type-II structures increase V_{oc}	Improved stability and photoluminescence; tunable band alignment	More complex synthesis; increased QD size may reduce loading density	115
QD loading optimization (secondary deposition/CLIS)	Increases QD surface coverage on TiO_2 scaffold and boosts light absorption	PCE improved from 13.54% → 15.31% in ZCISSe QDSCs through secondary deposition	Directly enhances J_{SC}; compatible with existing QDSSC platforms	Excessive loading can increase charge recombination; limited by pore filling	18
Band alignment engineering (ETM/HTM optimization)	Aligns conduction/valence bands to minimize interfacial energy loss and suppress dark current	Hybrid TiO_2/ZnO ETM raises PCE to 18.24%; spiro-OMeTAD achieves 23.14% V_{oc} boost	Enhances charge extraction efficiency and V_{oc} simultaneously	Requires precise energy-level matching; material-specific optimization needed	81
Plasmonic enhancement (Au/Ag nanoparticles)	Surface plasmon resonance (SPR) increases local electromagnetic field and photon absorption	PCE enhanced to 11.0% in PbS QDSCs using V-groove/parabolic light-trapping structures	Broadband absorption enhancement; synergistic with QD-based MEG	Metal nanoparticles may introduce recombination centers if improperly positioned	126
Multiple exciton generation (MEG) exploitation	Single high-energy photon generates multiple electron–hole pairs, surpassing Shockley–Queisser limit	Theoretical PCE up to 44.7%; external quantum efficiency >114% demonstrated in PbSe nanorods	Can fundamentally exceed single-junction efficiency limit; increases J_{SC}	Efficient carrier extraction remains difficult; Auger recombination competes strongly	99
AI/machine learning-assisted design	Data-driven optimization of materials, device geometry, and synthesis parameters	Accelerates device development and reduces experimental trial-and-error	Rapid screening of large parameter spaces; predictive stability modelling	Requires large, high-quality datasets; limited model interpretability	127

scaffolds. Band alignment engineering, particularly through hybrid TiO_2/ZnO electron transport layers, has yielded efficiencies of 18.24%, confirming that precise interfacial energy-level matching is among the highest-impact strategies for improving both charge extraction efficiency and open-circuit voltage simultaneously.[14,18,81]

Among the strategies evaluated, multiple exciton generation (MEG) exploitation and AI-assisted design represent the most transformative long-term approaches. MEG fundamentally challenges the Shockley–Queisser efficiency ceiling, with theoretical PCEs of up to 44.7% and demonstrated external quantum efficiencies exceeding 114% in PbSe nanorods; however, efficient carrier extraction at the device level remains a critical bottleneck that must be resolved before MEG can deliver practical efficiency gains. AI and machine learning-assisted optimization, while currently limited by dataset availability and model interpretability, offer the most promising route for accelerating QDSC development by enabling rapid screening of material combinations, device geometries, and synthesis parameters across all QD systems simultaneously. Collectively, the strategies outlined in Table 7 are most effective when applied in combination for example, pairing surface passivation with band alignment engineering or integrating plasmonic enhancement with MEG-active QD absorbers rather than as isolated interventions.[99]

7. Stability and degradation of QDSCs

Environmental factors and intrinsic material properties that impair device durability also shorten the operational lifespan of QDSCs. Better techniques for enhancing durability are developed when these degradation processes are fundamentally understood. When exposed to high temperatures and ambient air moisture, lead-chalcogenide and lead-halide perovskites exhibit vulnerability to oxidation and deterioration.[128] Without protection, the performance gradually deteriorates over time. When they interact with other cell layers, QD-based deterioration takes place. Over time, the MoO_2 interfacial layers' band alignment changes, reducing the device's stability.[129] The ligands selected for the material have a significant impact on QD stability. While inorganic ligands, like iodide, guard against air deterioration, ligands composed of organic materials are more susceptible to oxidation. QD degradation is the outcome of both chemical entities' surface binding. Because water molecules have a tendency to adhere to a particular surface, the degradation process accelerates in the presence of humidity.

QDSCs operational lifetime is shortened by exposure to high lighting levels since it results in light-based oxidation processes and thermal stress.[130,131] When used as sealing materials, glass and polymer films serve as barriers for devices that preserve the environment. Although engineering protective materials are effective, they add costs and challenges to the system. By repairing QD surface flaws, molecular coatings and self-healing materials offer oxidation resistance.[132] The use of stable ligands, ideal thicknesses, and the selection of low-reactivity materials yield the fundamental stability characteristics of devices. Stable performance measurements for various devices under various conditions are provided by standardized testing procedures that adhere to perovskite solar cell testing standards.[133] Effective encapsulation techniques and fixes for stability problems are necessary for QDSCs in order to guarantee their commercial viability.

8. Interface engineering and charge transport mechanism in QDSCs

The interface engineering is a convincing factor in the photovoltaic performance manner of QDSCs wherein the efficiency of the device is strongly related to efficient charge separation, transport and collection processes through internal interfaces.[134] Efficient carrier movement between quantum dot layers, charge transport layers and electrodes are critical aspects of high power conversion efficiency and poorly designed interfaces add trap states and recombination centers, limiting output of the devices.[135] Charge recombination at heterojunction interfaces and internal layers of quantum dots can be listed among the key drawbacks of QDSCs.[136] Whereas quantum dots have a high optical absorption and tunable bandgaps, interfacial losses have a severe effect, and the approaches to interfaces enhancement are of primary importance.[137] One of the approaches to enhancing the charge transport in QDSCs is band alignment engineering.[138] Appropriate alignment of the values of conduction and valence bands of energy levels at device interfaces leads to an improvement in open-circuit voltage, elimination of dark current losses, and directional carrier transfer. It has been demonstrated with theoretical research that optimized carrier mobility and interface energetics can contribute to photovoltaic performance to a large degree.[139] The architecture of the device and charge transport mechanism are represented in Fig. 21.

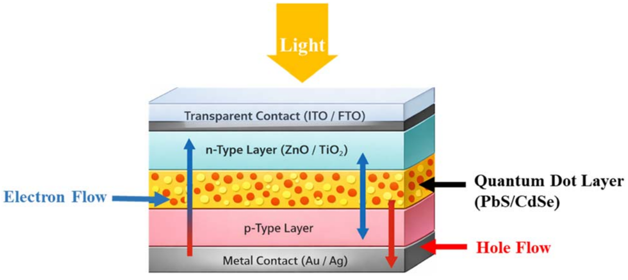


Fig. 21 An illustration of the charge transfers and device architecture of a QDSC. The n-type layer of the transport and the transparent electrode (as well as the metal contact) will receive electrons generated by photogeneration, whereas the p-type layer will receive holes.[11]

Heterojunction interfaces geometry and location can have a very pronounced effect on charge transport kinetics and device behavior of fill factor and hysteresis behavior.[140] It has been shown in experimental studies that transport on either side of interfaces of balanced electron and hole is critical to stabilized and effective work of QD based photovoltaic gadgets.[141] One of the efficient ways to reduce recombination losses is by means of passivation of the surface. The art of coating quantum dots with compatible shell materials enhances the surface electronic structure, elimination of traps states as well as increased long-term stability.[142] As an example, PbS quantum dots with a perovskite shell passivation can strongly inhibit the recombination process without degrading the device operation during a long time.[143] New direction current trends in research are on more complex methods of interface modification like ligand engineering, atomic layer deposited interlayers, graphene transport layers, and nanostructured blocking layers.[144] These approaches are meant to maximize interfacial energetics, minimize recombination, and maximize charge extraction efficiency, and interface engineering is one of the most important areas of the research emphasis of the next-generation QDSCs.[145]

9. Recent progress in QDSCs technologies

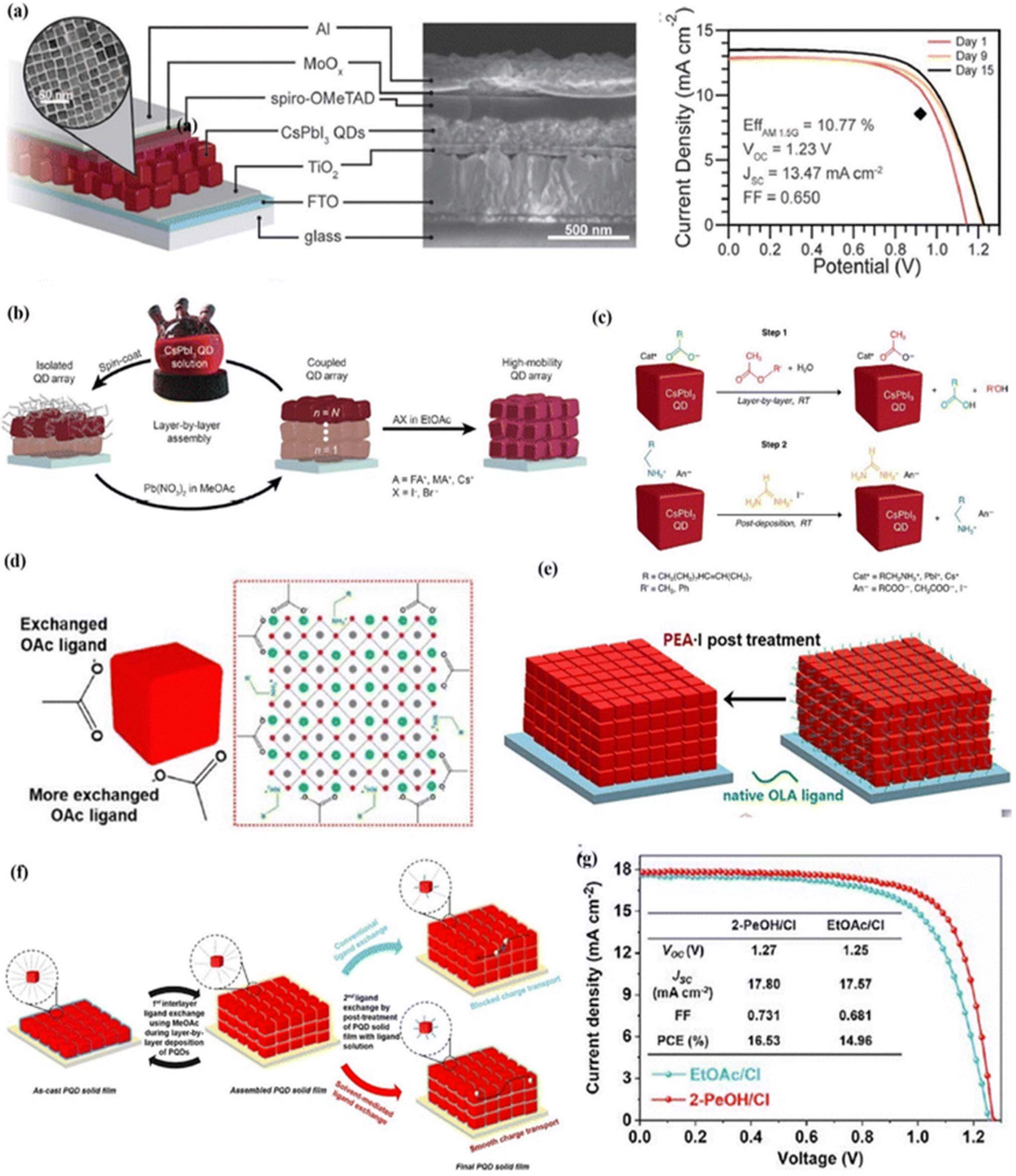
The field of QDSCs has made significant strides in material production, device development, and architectural advancements. Researchers have developed new technologies that solve issues with long-term stability and operational scale while addressing power efficiency limitations. According to research by ref. 146, core shell (CSQDSCs) offer adjustable bandgaps together with improved charge carrier dynamics, providing higher stability. This makes them an attractive technological platform. Better efficiency results are achieved by this core–shell design, which also reduces non-radiative recombination and corrects surface imperfections.[147] This technology is unable to achieve commercial success due to concerns of long-term stability, scalability, and material toxicity. For current research, scientists investigate novel lead-free materials and sophisticated passivation techniques. Broad spectrum quantum dot absorption is made possible using numerous layers that combine silicon-based components, perovskite materials, and quantum dot core–shell structures. This allows for the acquisition of the better efficiency features of additional materials. The efficiency potential of separate quantum dot solar units may be surpassed by such a combination of strategies. Luminescent solar concentrators (LSCs) have also emerged as a promising approach for building-integrated photovoltaics, wherein QDs serve as fluorescent absorbers that collect and redirect sunlight toward photovoltaic cells at the edges of a transparent waveguide. Recent advances in QD-based LSCs have demonstrated significant progress, with heavy-metal-free $CuInS_2/ZnS$ core–shell QDs achieving optical efficiencies of up to 26.5% owing to their large Stokes shift and high photoluminescence quantum yield. Ga-doped $CuInS_2$

QDs have further pushed photoluminescence quantum yields to 92%, substantially reducing reabsorption losses. Furthermore, all-perovskite LSC photovoltaic windows have been demonstrated with high optical transparency, highlighting the potential of QD-LSC systems for next-generation building-integrated and semi-transparent photovoltaic applications.[37,38] Together with synthesis techniques and device architecture, artificial intelligence and machine learning analyze vast amounts of experimental and simulation data to identify the optimal material mixes. This sophisticated procedure leads to both improved operational capabilities and efficient device development.[148] The highest certified power conversion efficiency recorded for QDSCs has reached 18.3% as of 2025, although theoretical models suggest that exploitation of MEG characteristics could enable a maximum efficiency of 44.7% under the intermediate band concept, and up to 66% under ideal quantum confinement conditions, highlighting the substantial gap that remains between current experimental achievements and the theoretical potential of this technology.[149] When used in conjunction with other solar cell technologies, QDSCs increase efficiency because they use quantum dots to catch light at a variety of wavelengths. By combining quantum dots with other solar cell technologies, solar cell efficiency can be higher than that of single-junction cells.[150]

According to research findings, CSQDSC coupled with silicon-based or perovskite layers offers a viable technological framework for advanced solar energy solutions.[151,152] A significant advancement in photovoltaic technology, QDSCs offer improved alternatives to conventional silicon-based solar cells.[17] QD optoelectronic properties, such as bandgap adjustment and additional excitation generating capabilities, are advantageous for sunlight harvesting.[41] The entire structure of QDSCs is composed of these basic components. This component provides the structure with physical support. Glass is used in various QDSC structures in conjunction with flexible polymers. Light can travel through the front electrode while electrons are being collected and transported at the same time. Indium tin oxide (ITO) and fluorine-doped tin oxide (FTO) are the two TCO materials most frequently used in solar cells[152] facilitate the transfer of electrons from the QDs to the TCO. Titanium dioxide (TiO_2) is a common choice for solar cell applications because of its strong electron mobility and proper energy level alignment.[153] The solar cells actively absorb light-absorbing components. Through photon absorption, electron–hole pairs are produced during the excitation process in quantum dots. Cadmium sulphide (CdS), cadmium selenide (CdSe), lead sulphide (PbS), and copper indium gallium selenide (CIGSe) are all used by the active materials in solar cells.[154] Through its attachment to the back electrode, the QD material makes use of transport holes. PEDOT:PSS and spiro-OMeTAD are two commonly utilized materials in this application. The electrical circuit's destination is the hole collector. Scientists select Au, Ag, or Pt as metals for the absorber layers based on the application. Through processes like polysulphide or iodide/triiodide medium acting as the electrolyte, the electrolyte system in QDSSCs permits both the flow of charges and QD recovery.[153] QDSC development has concentrated on the use of novel materials and device systems to improve stability and efficiency. Lead halide is one of the main areas of progress. Perovskites and other PQD materials show a lot of promise as photoactive materials due to the combination of their exceptional optoelectronic properties and straightforward production techniques. As seen in Fig. 22, surface engineering methods such as ligand exchange are required to maximize the operating performance of PQDs for solar cells. The efficiency of CDs for PQDSCs produced by alkyl ammonium iodide-based ligand exchange techniques is noticeably higher than that of their conventional inorganic counterparts.[155]

GQDs have strong conductivity and changeable band gaps because of their zero-dimensional carbon nanomaterial architecture. GQDs are advantageous when added to various solar cell layers for solar energy gathering.[152] Materials in the form of core nano-quantum dots encased in another semiconductor shell make up semiconductor structures. In addition to reduced surface defect presence, core–shell QDs provide improved quantum yield capabilities and enhanced stability properties.[156] Surface modification of QDs with appropriate ligands and treatments allows for improved charge transport functions and a reduction in non-radiative recombination occurrences. The binding of diamines to tin atoms in mixed Sn–Pb perovskite thin films increases stability by lowering oxidation processes and recombination frequencies. Similar to conventional QDSSCs work as solar cells by using QDs as light-absorbing sensitizers. Because three-dimensional electrodes produce more QD absorption sites and better charge transport mechanisms, they increase operational efficiency in QDSSCs.[157] A framework for overcoming the efficiency limitations of traditional single-gap solar cells is created by the theoretical concept of QD intermediate band solar cells (QD-IBSCs). The cells employ QD implementation in semiconductor materials to create an intermediate band to absorb photons with energy below the bandgap. A layer of perovskite quantum dot composite film serves as a luminescence downshifting (LDS) element to enhance the UV-blue spectrum response of silicon solar cells and increase their power conversion efficiency.[158]

QDSCs continue to confront difficulties despite the notable advancements. Although solar cell technologies employing alternative techniques maintain higher real efficiency levels, theoretical models show great efficiency. In addition to device structural designs, scientists need to conduct more research to refine QD structural elements and surface treatments.[49] QD materials are prone to deterioration when exposed to air and dampness. Since encapsulation and surface passivation are essential stability enhancers, they are crucial to the long-term stability of solar cells.[159] Lead and cadmium are among the hazardous substances found in several QD materials. Finding and creating eco-friendly quantum dot substitutes is a crucial step in the development of sustainable solar cell technology. The field's research should concentrate on developing tandem solar cell device designs, finding new quantum dot materials, and improving the stability and scalability of QDSC production.[160] Development of QDSC seeks to play a significant part in the development of solar power generation technologies in the future.[161]



	2-PeOH/Cl	EtOAc/Cl
V_{OC} (V)	1.27	1.25
J_{SC} (mA cm^{-2})	17.80	17.57
FF	0.731	0.681
PCE (%)	16.53	14.96

Fig. 22 PQD solar cells composition and functionality. (a) Device architecture, cross-sectional SEM image, and *J*–*V* characteristics of PQD solar cells. (b) Layer-by-layer assembly and cation/anion exchange for high-mobility PQD arrays. (c) Two-step ligand exchange mechanism using carboxylic acid and ammonium salts. (d) Enhanced acetate (OAc) ligand exchange on PQD surfaces. (e) PEA-I post-treatment for surface ligand modification and passivation. (f) Sequential interlayer and post-deposition ligand exchange strategy for improved charge transport. (g) *J*–*V* performance comparison of ligand-treated PQD solar cells.[32]

10. Challenges and prospects

Before QDSCs were extensively used as a profitable and sustainable technology, a few issues need to be resolved. Due to their heavy metal composition, which includes lead and cadmium, many QDs pose significant risks to both human health and the environment. Research papers state that scientists are employing carbon-based QDs, PQDs, and other non-toxic materials to create alternatives free of lead and cadmium.[148] Because it reduces environmental risks, proper QDSC disposal management and recycling initiatives must be put in place. The environmental risks associated with QD materials will be lessened by a recycling system that can handle them effectively. The limits of spin-coating in conjunction with layer-by-layer deposition fabrication techniques hinder the current mass-production scaling of quantum dots. Roll-to-roll printing and inkjet printing systems are two examples of cost-effective scalable techniques that must be developed for commercial application going forward.[162] Some studies highlight emerging interdisciplinary directions involving meta-materials, photothermal management, plasmonics, artificial intelligence-assisted optimization, and defect engineering, all of which may play crucial roles in overcoming the present limitations and advancing the next generation of high-performance and stable QDSCs.[163–167]

High precursor material costs and intricate production procedures that exceed the expenses of silicon-based photovoltaic cells limit the market potential of QDSCs. Optimizing their synthesis procedures and manufacturing infrastructure to lower production costs will be crucial to QDSCs commercial debut. Research on carbon-based quantum dots and perovskite quantum dots is broadening the areas of non-toxic alternatives.[168]

The materials have the potential to create sustainable, effective gadgets. When quantum dots and perovskite materials are combined in tandem devices, both technologies can take advantage of their unique capabilities to produce devices with better efficiency than single QDSCs. Combining these strategies offers a practical way to address the environmental issues and performance constraints that exist today.[169] By identifying the optimal patterns for device architecture and material combination, AI accelerates development cycles through data assessment.[51] By using this method, experimental trial-and-error attempts and the associated costs and timeframes would be reduced. By integrating new materials and technology, QDSCs will overcome their existing challenges and become commercially viable green solar energy systems.[62,170] The future QDSC technologies may significantly benefit from integrating photonic crystals, functional nanodots, two-dimensional materials, layered nanostructures, and bio-inspired photosensitive systems to achieve superior photovoltaic efficiency, long-term stability, and multifunctional device applications.[171–175]

11. Conclusion

QDSCs have become widely regarded as one of the most promising types of next-generation photovoltaic technologies that can offer special benefits not just as compared to the standard silicon-based solar cells. Their size-tunable quantum confinement can be used to provide broad spectral absorption, extraction of hot-carriers and creation of multiple excitons, with theoretical efficiencies of 66% and experimentally demonstrated efficiencies of more than 18%. In terms of light-harvesting and power conversion capacity, QDSCs are strong rivals to multi-junction devices due to the limited control over optical and electrical properties of quantum dots based on size, composition, and surface chemistry. By controlling nanocrystal size, surface passivation, and flaws, recent technologies in QD synthesis such as colloidal, hydrothermal, and chemical vapour deposition have improved charge transfer and reduced recombination losses. Further improvements in device stability and performance have been achieved through interface engineering, ligand exchange strategies and heterostructure designs that have shown the importance of nanoscale control in the efficiency of the quantum dots in addition to the progress of lead and cadmium-free quantum dots, perovskite-quantum dot hybrids and core–shell designs have also been developed to reduce environmental and health impacts, as well as improve the performance of quantum dots devices. Solution-based fabrication with low temperatures offer an alternative to traditional photovoltaic manufacturing methods with a lowered cost, scale, and sustainability. Wearable electronics, building-integrated photovoltaics, and automotive energy applications are all made possible by QDSCs inherent flexibility and excellent efficiency under a variety of illumination conditions. However, given the present problems with the high production volume, long-term stability, and toxicity of the materials that make up the QDSCs, more interdisciplinary research in the fields of materials science, interface engineering, and device architecture is probably going to result in the QDSCs maximum potential. As they continue to advance with innovation, environmentally benign design and increasingly become economically viable, QDSCs will be at the center of the future scenario of renewable energy with high performance and high sustainability and help in the world to go green and move towards circular energy technologies.

Conflicts of interest

There are no conflicts to declare.

Data availability

No primary research results, software or code have been included and no new data were generated or analysed as part of this review.

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