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MXene Quantum Dots as Multifunctional Interfacial Modulators for High-Performance Perovskite Solar Cells

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Abstract

MXene quantum dots (MQDs) are zero-dimensional derivatives of MXenes with unique physicochemical properties. Owing to their tunable surface chemistry, excellent conductivity, and abundant functional groups, MQDs have emerged as promising materials for perovskite solar cells (PSCs). Their unique combination of tunable surface chemistry, high electrical conductivity, and quantum-confined electronic properties enables multifunctional roles at interfaces and within perovskite films. MQDs can simultaneously act as defect passivators, band-alignment modulators, crystallization directors, and localized charge transport facilitators, collectively improving power conversion efficiency, reducing hysteresis, and enhancing operational stability. Incorporation strategies include integration into electron transport layers (ETLs), hole transport layers (HTLs), and perovskite precursors, where MQDs regulate nucleation and growth, optimize energy-level offsets, and mitigate interfacial recombination. Mechanistic studies reveal that surface terminations such as –O, –OH, –F, and –Cl are critical for achieving these multifunctional effects. Despite significant progress, challenges remain in scalable synthesis, controlled functionalization, and large-area device integration, particularly for flexible and tandem PSC architectures. Future directions involve combinatorial approaches that couple precise MQD design, advanced characterization, and computational modeling to fully exploit their potential. This review consolidates the current understanding of MQDs and provides a comprehensive perspective on their mechanistic, structural, and device-level impacts in PSCs. To the best of our knowledge, it is among the few reviews specifically focused on the roles of

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MQDs in PSCs, with particular emphasis on their integration pathways, interfacial functions, and effects on photovoltaic performance and stability.

Keywords: MXene quantum dots; Perovskite solar cells; Interface engineering; Defect passivation; Crystallization control; Charge transport

1. Introduction

Perovskite solar cells (PSCs) have rapidly emerged as one of the most promising photovoltaic technologies due to their high power conversion efficiencies (PCEs) and potentially low manufacturing costs.[1] Recent advances have pushed certified efficiencies above 25%, approaching the thermodynamic limits for single-junction devices [2]. However, intrinsic instability, high defect densities, and inefficient charge extraction at interfaces remain critical barriers to commercial deployment [3]. Defects in perovskite films and mismatches in energy levels at interfaces restrict efficient charge separation, leading to nonradiative recombination and device degradation [4].

To address these issues, extensive research has focused on interfacial and structural engineering, including passivation layers, compositional optimization, and interfacial dipole formation strategies that enhance charge extraction and reduce recombination losses [5]. Among the various techniques, quantum dot (QD) interface modification has attracted considerable attention for its ability to tailor local electronic structures and passivate defect states within PSC architectures.[6] QDs can optimize energy level alignment between adjacent layers and assist crystallization, facilitating improved charge transport and stability [7].

Within this context, MXene quantum dots (MQDs) – ultra-small fragments of two-dimensional transition metal carbides/nitrides – have recently emerged as a highly promising class of interfacial modifiers [8]. Unlike larger two-dimensional MXene nanosheets, MQDs possess high surface-to-volume ratios and abundant surface functional groups, facilitating stronger interactions with perovskite constituents and charge transport layers [9]. The unique combination of tunable energy levels, high conductivity, and rich chemistry enables MQDs to play multifunctional roles in optimizing PSC performance [10].

Initial studies on MQDs in PSCs demonstrated that integrating MQDs into electron transport layers (ETLs) significantly enhances band alignment, defect passivation, and film quality, ultimately leading to improved efficiency and stability [11]. For example, when incorporated into a SnO_2 ETL, MQDs were shown to lower trap state density, enhance charge transport, and increase the PCE from ~17.4% to ~21.6% compared to pristine SnO_2-based cells, while also improving ambient and thermal stability [12]. These improvements were attributed to the strong bonding between MQDs and both transport layer and perovskite constituents, effectively reducing interface recombination sites [13].

Beyond ETLs, MQDs have also been applied in dual-interface strategies, such as simultaneous modification of ETL/perovskite and perovskite/HTL interfaces, yielding enhanced charge extraction and reduced hysteresis in PSCs [14]. Such studies underscore the ability of MQDs to improve multiple device performance indicators through coordinated interface engineering [15].

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Another critical advantage of MQDs lies in their ability to modulate crystallization kinetics [16]. The presence of MQDs at the perovskite/ETL interface was found to induce rapid heterogeneous nucleation, forming intermediate perovskite phases during processing [17]. This effect promotes larger crystal grains, reduced trap states, and improved phase stability, which are fundamental for high-performance and long-term operational stability of PSCs [18].

Despite these advancements, several challenges persist [19]. Achieving controlled and reproducible MQD synthesis with desirable functional groups and electronic structures remains non-trivial [20]. Furthermore, optimal integration strategies that balance MQD concentration, spatial distribution, and surface termination in scalable device fabrication processes are yet to be fully established [21]. Addressing these issues is critical for realizing the full potential of MQDs in PSCs and translating laboratory-scale improvements into commercially viable technologies [22].

Despite the rapid progress in perovskite solar cells, challenges related to charge recombination, interface defects, and long-term operational stability still limit their large-scale commercialization. Recently, MQDs have emerged as promising nanomaterials for addressing these issues due to their unique properties, including high electrical conductivity, tunable surface chemistry, and abundant functional groups. Although several studies have explored the application of MXenes and quantum dots in photovoltaic devices, a comprehensive and systematic overview specifically focusing on MQDs in PSCs is still lacking. In particular, the multifunctional roles of MQDs in charge transport modulation, defect passivation, interface engineering, and stability enhancement have not been critically summarized in the existing literature. Given the rapidly increasing number of publications in this area over the past few years, a timely and comprehensive review is necessary to consolidate current knowledge, identify key technological challenges, and provide future research directions. Therefore, this review aims to systematically summarize the synthesis strategies of MQDs, their integration approaches in PSC architectures, and the mechanisms by which they improve device performance and stability.

The best of our knowledge, only limited review attention has been devoted specifically to the application of MQDs in PSCs. In contrast to broader reviews on MXene-based materials, quantum dots, or interfacial engineering in perovskite photovoltaics, the present review focuses specifically on MQD-enabled strategies in PSCs, including their synthesis, physicochemical characteristics, interfacial roles, and effects on charge transport, defect passivation, efficiency, and stability. While several recent review articles have addressed MXene-derived materials, nanostructured interfacial modifiers, or quantum dot-assisted optimization in PSCs, a dedicated review centered specifically on MQDs and their multifunctional roles in PSCs remains limited. Accordingly, this article aims to provide a focused and integrative overview of this emerging topic [23-30].

2. Fundamental Properties and Synthesis of MXene Quantum Dots

This section reviews the main synthetic strategies used to produce MXene quantum dots and discusses how these approaches influence their structural and chemical properties. The section

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first describes commonly used preparation routes, including top-down exfoliation and chemical fragmentation methods. It then examines how processing parameters affect MQD size distribution, surface terminations, and structural stability. Understanding these synthesis pathways is essential because the resulting physicochemical characteristics of MQDs strongly influence their behavior in photovoltaic applications.

MXenes represent a rapidly expanding family of two-dimensional (2D) transition metal carbides, nitrides, and carbonitrides with a general formula of $M_{n+1}X_nT_x$, where *M* denotes an early transition metal (e.g., Ti, V, Nb), *X* is carbon and/or nitrogen, and T_x represents surface terminations such as –O, –OH, –F, or –C [31, 32]. Since their first report in 2011, MXenes have attracted significant attention due to their metallic conductivity, hydrophilicity, tunable surface chemistry, and compatibility with solution-based processing. When MXenes are downsized into zero-dimensional (0D) structures with lateral dimensions typically below 10 nm, they are referred to as MQDs. This quantum-confined form introduces distinct optical, electronic, and interfacial properties that are fundamentally different from their bulk or 2D counterparts, making them particularly attractive for optoelectronic applications, including PSCs [33].

2.1. Structural and Electronic Characteristics of MXene Quantum Dots

MQDs inherit the layered atomic structure of their parent MXenes but exhibit pronounced quantum confinement and edge effects due to their nanoscale dimensions. The reduced size leads to discretization of energy levels, resulting in size-dependent band structures and optical transitions [34]. Unlike bulk MXenes, which often show metallic or semi-metallic behavior, MQDs can display tunable semiconducting characteristics with finite bandgaps, typically ranging from ~1.5 to 3.5 eV depending on composition, size, and surface terminations. This transition from metallic to semiconducting behavior is a critical feature enabling their integration into photovoltaic architectures where energy-level alignment is essential [35, 36].

The electronic structure of MQDs is strongly influenced by surface terminations. Density functional theory (DFT) calculations and spectroscopic studies have demonstrated that –O and –OH terminations generally induce wider bandgaps and stronger dipole moments compared to –F terminations. These surface dipoles play a crucial role in modulating local electric fields at interfaces, which is particularly beneficial for charge extraction and recombination suppression in PSCs. Additionally, the high density of edge sites in MQDs provides abundant active sites for interfacial interactions, defect passivation, and chemical bonding with adjacent layers [37, 38].

The schematic in panel (a) figure 1 illustrates a multi-step synthesis route for $Ti_3C_2T_x$ MQDs, starting from the MAX phase precursor Ti_3AlC_2. This process involves selective etching with HCl/LiF to remove the Al layers, yielding multilayer MXene (m-$Ti_3C_2T_x$), followed by ultrasonication for delamination into few-layer sheets (d-$Ti_3C_2T_x$), and culminating in a hydrothermal treatment to fragment these into quantum dots. This approach exemplifies the top-down fabrication typical for MQDs, preserving the inherent hydrophilicity and surface functional groups of MXenes while enabling size control at the nanoscale, which aligns with the solution-processable nature of these materials for integration into optoelectronic devices. Panel (b) presents a transmission electron microscopy (TEM) image revealing the uniform dispersion of

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MQDs with diameters ranging from 1.6 to 4.0 nm, emphasizing their homogeneous morphology. The magnified view in panel (c), along with the corresponding line profile and high-resolution TEM (HRTEM), confirms an interplanar spacing of 0.21 nm attributable to the (0110) planes, indicative of the preserved crystalline structure from the parent MXene. These observations underscore the quantum confinement effects arising from the sub-10 nm lateral dimensions, which discretize energy levels and introduce edge-dominated properties, enhancing their suitability for applications requiring precise interfacial control.

High-resolution X-ray photoelectron spectroscopy (XPS) spectra in panels (d) and (e) detail the O 1s and F 1s regions, respectively, highlighting the surface terminations critical to MQD functionality. The O 1s peaks at 529.2 eV (Ti-O), 531.8 eV (Ti-OH), and 533.2 eV (adsorbed water) demonstrate the presence of oxygen-based groups, while the F 1s signals at 684.8 eV (Ti-F) and 686.1 eV (Al-F_x byproduct) confirm fluorine terminations. Such terminations, as evidenced here, modulate the electronic structure by influencing dipole moments and bandgap tuning, supporting the semiconducting behavior observed in MQDs compared to metallic bulk MXenes. The UV-vis absorption spectrum in panel (f) shows distinct edges at approximately 272 nm and 332 nm for the MQD aqueous solution, contrasting with the broad, plasmonic response of d-$Ti_3C_2T_x$. This shift is attributable to quantum confinement, where the reduced dimensionality widens the bandgap and alters optical transitions, enabling tunable light absorption. Complementing this, the photoluminescence (PL) spectra in panel (g) exhibit excitation-dependent emission, with peaks intensifying and blue-shifting as excitation wavelengths decrease from 320 to 440 nm, reflecting the influence of surface states and size uniformity on emissive properties. Collectively, these characterizations validate the successful downsizing of MXenes into MQDs, where the retained layered structure combined with emergent quantum effects yields materials with enhanced optoelectronic tunability. The observed surface chemistry and optical responses facilitate energy-level alignment and defect passivation, reinforcing their potential in solar cells systems and by promoting efficient charge dynamics at interfaces without compromising the intrinsic advantages of 2D MXenes.

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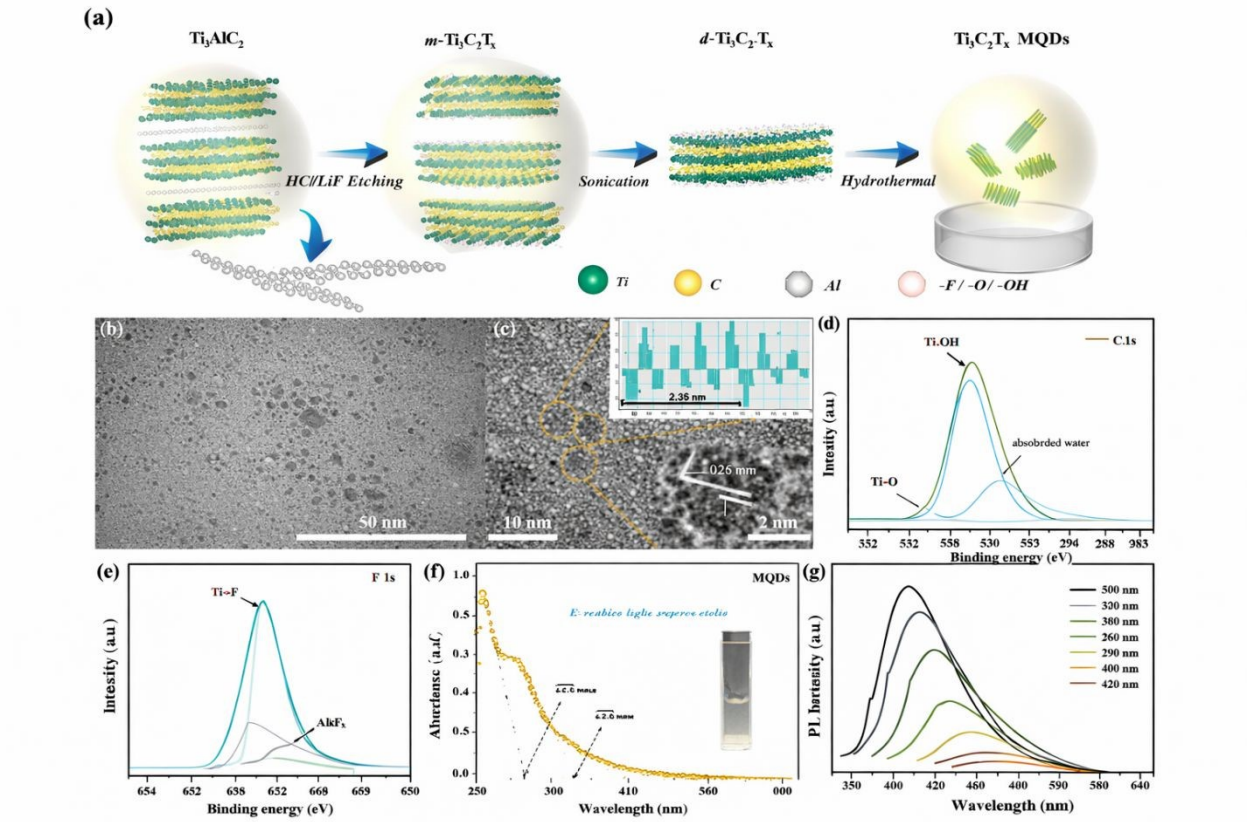

Figure 1. Synthesis and characterization of $Ti_3C_2T_x$ MQDs. (a) Schematic of the preparation process from Ti_3AlC_2 via HCl/LiF etching, sonication, and hydrothermal treatment. (b) TEM image of uniform MQDs (1.6–4.0 nm). (c) HRTEM with lattice spacing of 0.21 nm. (d,e) High-resolution XPS spectra of O 1s and F 1s confirming –O, –OH, and –F terminations. (f) UV-vis absorption spectrum showing bands. (g) Excitation-dependent PL spectra exhibiting blue-shifted and intensified emission. Adapted with permission from Ref. [80]. © 2023 Elsevier B.V.

2.2. Optical Properties and Quantum Confinement Effects

One of the most distinctive features of MQDs is their unique optical behavior arising from quantum confinement. MQDs typically exhibit strong absorption in the ultraviolet and visible regions, along with photoluminescence (PL) emission that is highly dependent on particle size, excitation wavelength, and surface chemistry. This excitation-dependent PL behavior is commonly attributed to a combination of quantum size effects and surface/edge states introduced by functional groups and structural defects [39].

The photoluminescence of MQDs is particularly relevant for photovoltaic applications, as it provides insights into charge recombination dynamics and defect states. Low PL intensity and shortened carrier lifetimes often indicate efficient charge transfer when MQDs are coupled with perovskite layers. Furthermore, the optical absorption of MQDs can complement the absorption spectrum of perovskite materials, potentially contributing to enhanced light harvesting when incorporated as interfacial modifiers or functional additives [40].

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An important characteristic of MXene quantum dots is the emergence of quantum confinement effects when the lateral dimensions of the material are reduced to the nanometer scale. At this scale, the electronic structure becomes size-dependent, leading to modifications in the density of states and band structure compared with bulk or layered MXene materials. These confinement effects can influence optical absorption, charge carrier dynamics, and surface reactivity. As a result, MQDs may exhibit tunable electronic and optoelectronic properties that are particularly advantageous for photovoltaic applications, where efficient charge transfer and defect passivation are critical for improving device performance.

2.3. Surface Chemistry and Chemical Tunability

Surface chemistry is a defining feature of MQDs and one of the primary reasons for their versatility in device engineering. The presence of abundant surface terminations enables strong chemical interactions with organic and inorganic materials. These functional groups not only influence solubility and dispersion stability in polar solvents but also allow MQDs to act as Lewis bases or acids, depending on their termination chemistry [41].

In the context of PSCs, the Lewis basic nature of oxygen-containing terminations (–O, –OH) is particularly advantageous for passivating undercoordinated Pb^{2+} ions at perovskite grain boundaries and interfaces. This chemical passivation reduces trap-assisted nonradiative recombination and enhances device stability [42]. Moreover, the surface chemistry of MQDs can be further engineered through post-synthesis treatments, such as thermal annealing, chemical functionalization, or ligand exchange, enabling precise control over their electronic and interfacial properties.

2.4. Synthesis Strategies for MXene Quantum Dots

The synthesis of MQDs generally involves a top-down or bottom-up approach, with top-down methods being more widely reported due to their simplicity and scalability. Top-down synthesis typically starts from bulk or few-layer MXenes, which are first prepared by selective etching of the "A" element from MAX phases (e.g., Ti_3AlC_2) using etchants such as HF, LiF/HCl, or other fluoride-based systems. Subsequent exfoliation yields few-layer MXene nanosheets, which are then broken down into quantum dots through physical or chemical means [43, 44].

Hydrothermal and solvothermal cutting are among the most common top-down techniques for MQD synthesis. In this method, MXene nanosheets are subjected to high temperature and pressure in aqueous or organic solvents, leading to oxidative cutting along defect sites and edges. Reaction parameters such as temperature, time, pH, and oxidant concentration play critical roles in determining the size distribution, crystallinity, and surface chemistry of the resulting MQDs. Typically, hydrothermal treatment at temperatures between 120–200 °C for several hours yields MQDs with diameters of 2–8 nm and good crystallinity [45, 46].

Ultrasonication-assisted exfoliation and cutting is another widely used approach. Prolonged sonication of MXene dispersions can induce cavitation forces that fragment nanosheets into quantum dots. While this method is straightforward and does not require harsh chemicals, it often results in broader size distributions and a higher density of defects. Nevertheless, these

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defects and edge states can be beneficial for interfacial interactions in photovoltaic devices [47, 48].

Bottom-up synthesis approaches, though less common, offer greater control over size and composition. These methods typically involve the direct nucleation and growth of MQDs from molecular precursors under controlled conditions. For example, solvothermal reactions using metal salts and carbon/nitrogen sources have been explored to synthesize Ti-based MQDs with tailored stoichiometry [49]. However, bottom-up approaches often face challenges related to phase purity, reproducibility, and scalability, which currently limit their widespread adoption (Figure 2).

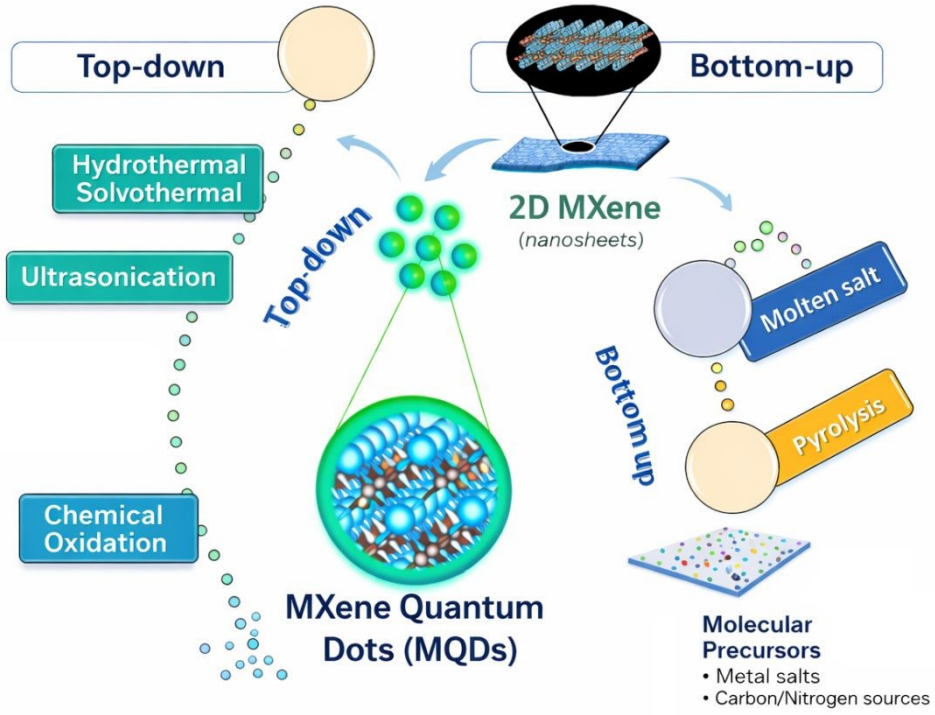

Figure 2. Schematic representation of top-down and bottom-up synthesis strategies for MQDs. Top-down methods convert 2D MXene nanosheets into MQDs via hydrothermal/solvothermal treatment, ultrasonication, or chemical oxidation, whereas bottom-up approaches involve direct MQD formation from molecular precursors through molten-salt processing or pyrolysis.

Table 1 summarizes representative synthesis routes for MQDs and highlights the trade-offs among process complexity, size control, surface terminations, and scalability. In general, top-down approaches are more compatible with established MXene processing routes and offer better prospects for scalable production, although they may introduce structural defects or partial oxidation depending on the cutting mechanism. By contrast, bottom-up methods generally provide finer control over MQD size and composition, but their broader implementation is still limited by challenges related to phase purity, reproducibility, and scale-up. Importantly, the synthesis conditions strongly affect the dominant surface terminations, which in turn influence the electronic structure, interfacial interactions, and device functionality of MQDs. Therefore, the choice of synthesis strategy should be determined not only by target particle size, but also by the desired surface chemistry and intended integration pathway in optoelectronic devices.

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Table 1. Representative synthesis strategies for MQDs and their main characteristics

Synthesis route	Starting material	Typical process conditions	Typical size (nm)	Dominant surface terminations	Main advantages	Main limitations
Hydrothermal cutting (top-down)	Few-layer MXene nanosheets (e.g., $Ti_3C_2T_x$)	120–200 °C, 6–24 h, aqueous or mixed solvents, controlled pH and/or oxidants	2–8	–O, –OH (with partial oxidation)	Narrow size distribution; good crystallinity; scalable process	Possible oxidation; sensitive to reaction duration
Solvothermal cutting (top-down)	Delaminated MXene flakes	140–220 °C in organic solvents (e.g., DMF, ethanol) under sealed conditions	3–10	–O, –OH, solvent-derived groups	Better control over surface chemistry; improved dispersion	Higher cost; solvent removal/post-treatment required
Ultrasonication-assisted exfoliation	Multilayer MXene powders	High-power sonication for 2–12 h under ambient or ice-bath conditions	3–15	–O, –OH, –F	Simple; low-cost; no harsh chemical oxidants	Broad size distribution; relatively high defect density
Chemical oxidation cutting	MXene nanosheets	Mild oxidants (e.g., H_2O_2, $KMnO_4$), room temperature to 80 °C	2–6	Oxygen-rich terminations	Rapid synthesis; relatively precise size control	Risk of over-oxidation; possible structural degradation
Bottom-up solvothermal synthesis	Metal salts with C/N-containing precursors	160–240 °C, inert atmosphere, 6–48 h	2–5	Tunable; ligand-dependent	Fine control over size and composition	Limited scalability; phase-purity challenges
Electrochemical exfoliation/cutting	Bulk MAX phase or MXene electrodes	Controlled voltage/current in suitable electrolytes	3–10	–O, –OH, –F (electrolyte-dependent)	Green route; low chemical waste	Equipment complexity; reproducibility

2.5. Structural Stability and Environmental Robustness

A critical consideration for MQDs is their structural and chemical stability, particularly under ambient conditions. Compared to bulk MXenes, MQDs often exhibit enhanced resistance to oxidation due to their smaller size and more uniform surface terminations. Nevertheless, oxidation remains a concern, especially for Ti-based MQDs, which can gradually transform into TiO_2 under prolonged exposure to oxygen, moisture, or light [50].

Surface functionalization and encapsulation strategies have been developed to mitigate degradation. For instance, controlling the ratio of –O to –OH terminations, incorporating antioxidant molecules, or embedding MQDs within polymer or inorganic matrices can significantly improve their environmental stability [51]. From a device perspective, even partially oxidized MQDs may retain beneficial electronic properties, such as suitable energy levels and defect passivation capability, which can still contribute positively to PSC performance.

2.6. Energy-Level Alignment and Charge Transport Properties

The energy-level structure of MQDs is a key parameter for their integration into PSCs. Ultraviolet photoelectron spectroscopy (UPS) and cyclic voltammetry measurements have shown that the work function and conduction/valence band positions of MQDs can be tuned over a wide

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range by adjusting composition, size, and surface terminations. This tunability allows MQDs to function as effective interfacial layers for either electron or hole extraction [52].

In addition to energy-level alignment, MQDs exhibit relatively high charge carrier mobility compared to many conventional quantum dots, owing to their inorganic nature and delocalized electronic states. Although charge transport in MQD films is often limited by inter-dot coupling and surface states, their role in PSCs is primarily interfacial rather than as bulk transport layers [53]. In this context, even moderate conductivity combined with favorable band alignment can substantially reduce interfacial resistance and enhance charge extraction efficiency.

2.7. Relevance of Fundamental Properties to Photovoltaic Applications

The unique combination of quantum confinement, tunable surface chemistry, and favorable electronic properties positions MQDs as highly promising functional materials for PSCs. Their ability to simultaneously modulate energy-level alignment, passivate defects, and influence interfacial electric fields distinguishes them from conventional organic or inorganic quantum dots. Importantly, these advantages are rooted in the fundamental properties discussed above, highlighting the critical link between synthesis, structure, and device functionality [54]. MQDs represent a distinct class of zero-dimensional materials with properties that can be precisely engineered through compositional control and synthesis strategies. Understanding their fundamental structural, optical, electronic, and chemical characteristics is essential for rational design and optimization in PSCs [55, 56].

3. Interface Engineering and Performance Enhancement Using MXene Quantum Dots

This section summarizes the principal techniques used to characterize MXene quantum dots and evaluate their structural, chemical, and electronic properties. The discussion covers microscopic, spectroscopic, and optical characterization methods that provide insights into MQD morphology, composition, surface chemistry, and electronic structure. These characterization approaches are essential for understanding how MQD properties relate to their functional roles in photovoltaic systems and for establishing reliable correlations between material structure and device performance.

Interface engineering has become a cornerstone in the design and optimization of advanced optoelectronic and energy-conversion devices, as interfaces often dictate overall performance more strongly than the intrinsic properties of the individual functional layers [57, 58]. In multilayer thin-film systems, charge generation, transport, and recombination processes are highly sensitive to the physical, chemical, and electronic characteristics of interfaces. Even when high-quality bulk materials are employed, poorly engineered interfaces can introduce severe efficiency losses, instability, and performance variability [59]. As a result, rational strategies that enable precise interfacial control are essential for the development of high-performance and reliable devices.

MQDs have recently emerged as a versatile class of interfacial materials capable of addressing multiple interfacial challenges simultaneously [60, 61]. Their zero-dimensional geometry, combined with rich and tunable surface chemistry as well as electronically active surfaces,

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enables MQDs to interact with neighboring materials at the atomic and molecular levels. Unlike conventional bulk additives or transport layers, MQDs primarily function as interfacial functional entities, exerting their influence locally while leaving the bulk properties of adjacent layers largely unaffected [62]. This characteristic makes them particularly attractive for interface-dominated device architectures, where subtle nanoscale modifications can translate into macroscopic performance improvements. Rather than fulfilling a single role, MQDs offer a multifunctional interface-engineering platform. They can regulate defect states, modulate interfacial energetics, redistribute charge density, and tailor local electric fields concurrently [63]. This multifunctionality clearly distinguishes MQDs from traditional molecular interlayers, self-assembled monolayers, or two-dimensional materials, which often address only one specific aspect of interfacial optimization.

3.1. General Interfacial Challenges in Multilayer Thin-Film Systems

Interfaces in heterogeneous thin-film structures are intrinsically complex regions where structural, electronic, and chemical discontinuities coexist. Lattice mismatch between adjacent layers can induce strain and structural defects, while differences in bonding configuration and surface chemistry result in dangling bonds or undercoordinated atoms [64]. These imperfections generate localized electronic states that act as charge trapping centers and facilitate nonradiative recombination processes, significantly degrading charge carrier utilization efficiency. The impact of such interfacial trap states on carrier losses is commonly described by the classical Shockley–Read–Hall recombination model:

$$R_{\mathrm{SRH}} = \frac{np - n_i^2}{\tau_p (n + n_1) + \tau_n (p + p_1)} \tag{1}$$

Where n and p are electron and hole concentrations, τ_n and τ_p denote carrier lifetimes, and n_1 and p_1 are parameters related to trap energy levels.

In parallel, unfavorable energy-level alignment at interfaces can lead to the formation of injection or extraction barriers, promoting charge accumulation and increasing resistive losses [65]. Such effects are particularly detrimental in thin and flexible devices, where interfaces account for a substantial fraction of the active region. Traditional interface-engineering strategies—such as plasma treatments, polymer buffer layers, or molecular self-assembled monolayers—often mitigate only isolated interfacial issues and may suffer from limited stability or scalability [66]. In contrast, MQDs provide a multidimensional toolbox that enables simultaneous chemical, electronic, and electrostatic modulation.

3.2. Defect Regulation and Chemical Passivation at Interfaces

A defining contribution of MQDs to interface engineering is their ability to regulate interfacial defect states through strong chemical interactions. MQDs possess a high density of surface functional groups, particularly oxygen- and hydroxyl-based terminations, which can coordinate with undercoordinated atoms and dangling bonds at material surfaces [67]. These interactions

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effectively neutralize deep electronic trap states that would otherwise serve as nonradiative recombination centers.

Beyond chemical passivation, the ultrasmall dimensions of MQDs allow them to physically occupy nanoscale voids and discontinuities at interfaces, resulting in improved surface conformity and reduced interfacial roughness. This physical filling effect minimizes local electric-field inhomogeneity and suppresses defect clustering, which is especially beneficial in polycrystalline and structurally heterogeneous systems [68]. The coexistence of chemical and physical passivation mechanisms enables MQDs to address interfacial disorder more comprehensively than conventional passivation layers.

3.3. Modulation of Interfacial Energetics and Local Electric Fields

Energy-level alignment across interfaces is a key determinant of charge transport efficiency in layered materials. MQDs offer exceptional flexibility in modulating interfacial energetics due to their size-dependent electronic structure and surface-induced dipole moments [69]. When introduced at an interface, MQDs can generate localized interfacial dipoles that shift the local vacuum level, a phenomenon commonly described by the relation:

$$\Delta E_{\mathrm{vac}} = \frac{e\,\mu_{\perp}}{\varepsilon_0 \varepsilon_r} \tag{2}$$

Where $\mu_{\perp}$ is the dipole moment normal to the interface, ε_0 is the vacuum permittivity, and ε_r is the relative dielectric constant of the interfacial environment. Such dipole-induced energetic modulation can reduce interfacial barriers, suppress charge accumulation, and promote directional charge transfer. Importantly, this effect is highly localized, enabling precise interfacial control while preserving the intrinsic properties of the surrounding materials. Compared to bulk doping or thick interlayers, this approach minimizes unintended side effects such as increased scattering or chemical instability [70].

3.4. Facilitation of Interfacial Charge Transfer

Efficient charge transfer across interfaces requires not only favorable energetic alignment but also sufficient electronic coupling. MQDs can facilitate interfacial charge transfer by acting as electronic bridges that provide intermediate energy states or enhance wavefunction overlap between adjacent layers [71]. Charge transport in the vicinity of interfaces is commonly described by the classical drift–diffusion equation:

$$J = qn\,\mu E + qD\nabla n \tag{3}$$

Where J is the current density, μ is the carrier mobility, E is the local electric field, and D is the diffusion coefficient. The presence of MQDs can locally modify both electric fields and carrier concentration gradients, thereby reducing interfacial charge transfer resistance and suppressing recombination losses. Although MQDs are not intended to function as long-range charge

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transport layers, their localized presence at interfaces can significantly improve charge transfer kinetics.

3.5. Influence on Interfacial Morphology and Structural Coherence

Interfacial morphology strongly influences mechanical adhesion, thermal robustness, and long-term reliability of multilayer thin-film systems [72]. The ultrasmall size and high surface activity of MQDs enable conformal coverage of rough or irregular surfaces, improving interfacial contact and reducing stress concentration points. This improved structural coherence enhances resistance to delamination and mechanical fatigue, which is critical for flexible and mechanically dynamic devices [73, 74]. Additionally, MQDs can influence nucleation and growth behavior of adjacent layers during deposition, indirectly affecting interfacial crystallinity and grain connectivity. These structure-directing effects further emphasize the active role of MQDs in shaping interfacial architecture rather than serving as passive modifiers [75, 76].

3.6. Interfacial Stability and Suppression of Degradation Pathways

Interfaces frequently act as initiation sites for chemical and electrochemical degradation driven by ion diffusion, redox reactions, or environmental exposure [77]. MQDs can enhance interfacial stability by forming chemically robust interlayers that block undesirable species migration and mitigate interfacial reactions. Their strong binding affinity and adaptable surface chemistry facilitate the formation of stable interfacial networks that resist chemical attack and mechanical delamination [78, 79]. This stabilization effect is particularly relevant under electrical bias, illumination, or thermal stress, where interfacial degradation often dictates operational lifetime. By suppressing these degradation pathways, MQDs contribute to improved durability and long-term reliability of multilayer devices.

MQDs can play multiple roles at critical interfaces in multilayer thin-film devices, particularly in perovskite solar cells. As illustrated in Figure 3, MQDs positioned at interfacial regions contribute to several synergistic mechanisms that enhance device performance. First, MQDs passivate surface and grain-boundary defects through chemical interactions with undercoordinated ions, thereby reducing trap-assisted recombination. Second, their surface functional groups can induce interfacial dipoles that help tune energy-level alignment between adjacent layers, facilitating more efficient charge extraction. MQDs also act as conductive bridges that accelerate interfacial charge transfer while suppressing carrier recombination. Additionally, they can improve interfacial morphology and film uniformity, and enhance environmental stability by mitigating ion migration and moisture-induced degradation.

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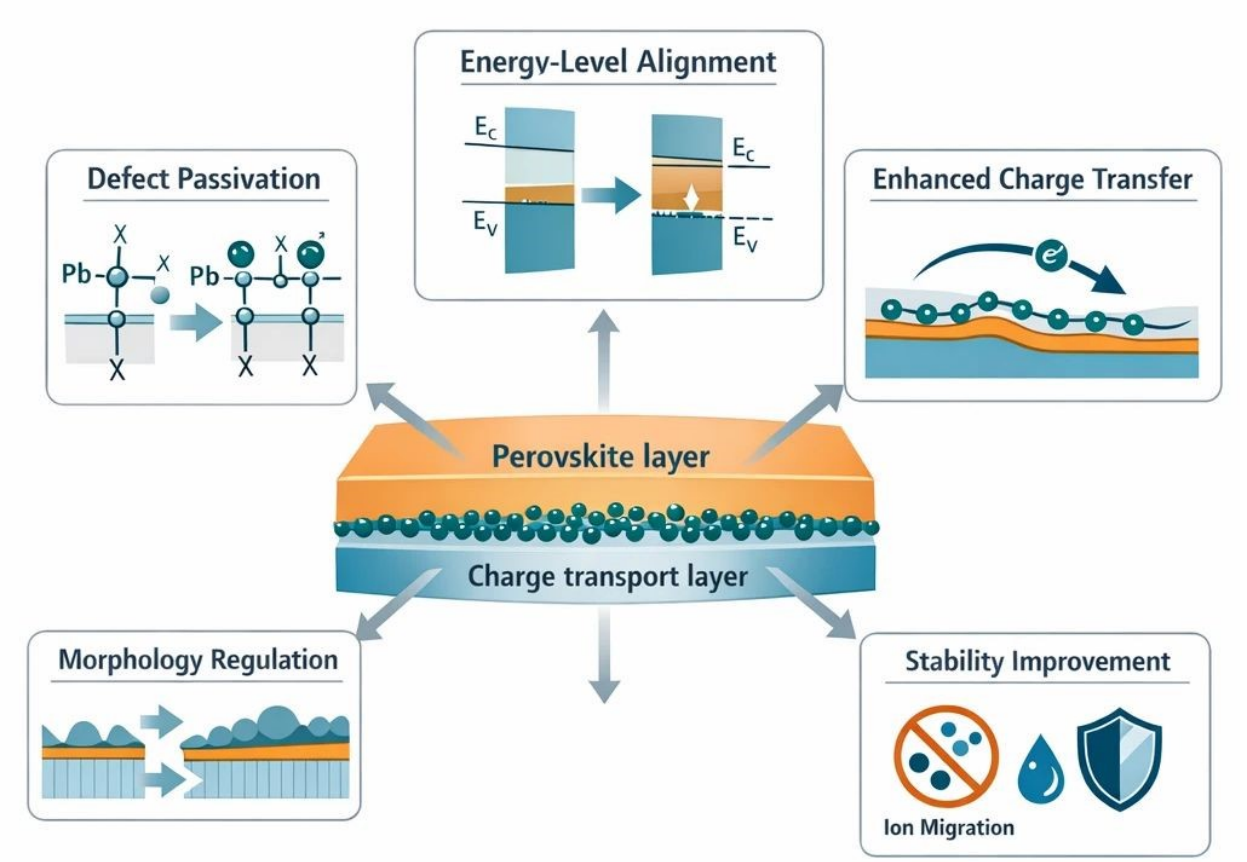

Figure 3. Conceptual schematic of multifunctional interface engineering enabled by MQDs, illustrating defect passivation, energy-level alignment, charge-transfer enhancement, morphology regulation, and stability improvement.

4. Application of MXene Quantum Dots in Perovskite Solar Cells

This section examines the different strategies used to integrate MXene quantum dots into perovskite solar cells and evaluates their influence on device performance. The discussion first considers the incorporation of MQDs in charge-transport layers, followed by their role in regulating perovskite crystallization and passivating defects. It then addresses interfacial energy-level engineering and charge transfer enhancement. Finally, an integrated assessment of the advantages and remaining limitations of MQD-based strategies is presented to highlight current challenges and future research directions.

The rapid progress of PSCs has been accompanied by growing recognition that device performance and stability are strongly governed by interfacial phenomena and crystallization dynamics rather than solely by bulk perovskite properties. In this context, MQDs have emerged as a highly adaptable functional material that can be strategically integrated into different components of PSC architectures. Unlike conventional additives or interlayers with a single dominant role, MQDs demonstrate multifunctional behavior, simultaneously influencing charge transport layers, perovskite film formation, interfacial energetics, and environmental stability.

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This section systematically analyzes the practical application of MQDs in PSCs based on experimentally validated strategies and mechanisms.

4.1. MQD-Modified Electron Transport Layers: Conductivity and Energy-Level Optimization

One of the earliest and most effective applications of MQDs in PSCs is their incorporation into ETLs, particularly metal oxides such as SnO_2 and TiO_2. The introduction of MQDs into ETLs addresses two intrinsic limitations of oxide-based transport layers: moderate electrical conductivity and suboptimal energy-level alignment with perovskite absorbers. When MQDs are embedded into SnO_2 ETLs, they significantly enhance electrical conductivity by introducing additional conductive pathways and reducing trap-assisted scattering within the oxide matrix [80]. More importantly, MQDs modify the interfacial electronic structure between the ETL and perovskite, resulting in improved band alignment that facilitates electron extraction while suppressing interfacial recombination. This dual improvement leads to a pronounced reduction in device defect density by nearly one order of magnitude, directly translating into enhanced charge transport and reduced nonradiative recombination losses.

Panel (a) in figure 4 presents a schematic energy band diagram for perovskite solar cells (PSCs) comparing pristine SnO_2 and MQD-modified SnO_2 electron transport layers (ETLs). The incorporation of MQDs shifts the conduction band of SnO_2 upward, achieving superior alignment with the perovskite absorber layer. This optimization reduces energy barriers for electron extraction toward the ITO electrode while enhancing hole-blocking capability at the ETL/perovskite interface, directly addressing the suboptimal band matching and moderate conductivity typical of metal oxide ETLs. Panel (b) displays steady-state photoluminescence (PL) spectra of perovskite films on SnO_2 and MQD-SnO_2 substrates. Contrary to common quenching observations, the MQD-modified film shows intensified PL emission, indicating significantly reduced nonradiative recombination within the perovskite and at the interface. This enhancement arises from improved perovskite crystallinity and fewer defects, facilitated by MQDs providing additional nucleation sites and conductive pathways that promote efficient charge separation.

In panel (c), time-resolved PL (TRPL) decay curves reveal a substantially prolonged average carrier lifetime for the MQD-SnO_2-based perovskite film (from ~67 ns to ~134 ns compared to pristine SnO_2). The slower decay dynamics confirm suppressed trap-assisted recombination and improved charge transport, reflecting the role of MQDs in passivating defects in the perovskite bulk, grain boundaries, and ETL interface through their abundant surface active sites. Panel (d) illustrates transient absorption (TA) decay kinetics at the photobleaching peak (~770 nm), fitted with double-exponential functions. The MQD-modified sample exhibits faster time constants for both electron injection (τ_1 reduced from 8.75 ps to 6.98 ps) and recombination processes, demonstrating accelerated charge transfer to the ETL and reduced defect-mediated recombination, consistent with lowered trap states and enhanced interfacial electronic structure.

Panel (e) shows current-voltage characteristics from space-charge-limited current (SCLC) measurements on electron-only devices, revealing a dramatic reduction in trap-filled limit voltage (V_{TFL} from 0.469 V to 0.058 V) and trap density (N_t from ~5.2×10^{21} cm^{-3} to ~6.4×10^{20}

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cm^{-3}) upon MQD incorporation into SnO_2. This near-order-of-magnitude defect density decrease, combined with improved conductivity via additional pathways within the oxide matrix, underscores how MQDs simultaneously optimize energy-level alignment and electrical transport, leading to minimized nonradiative losses and superior photovoltaic performance.

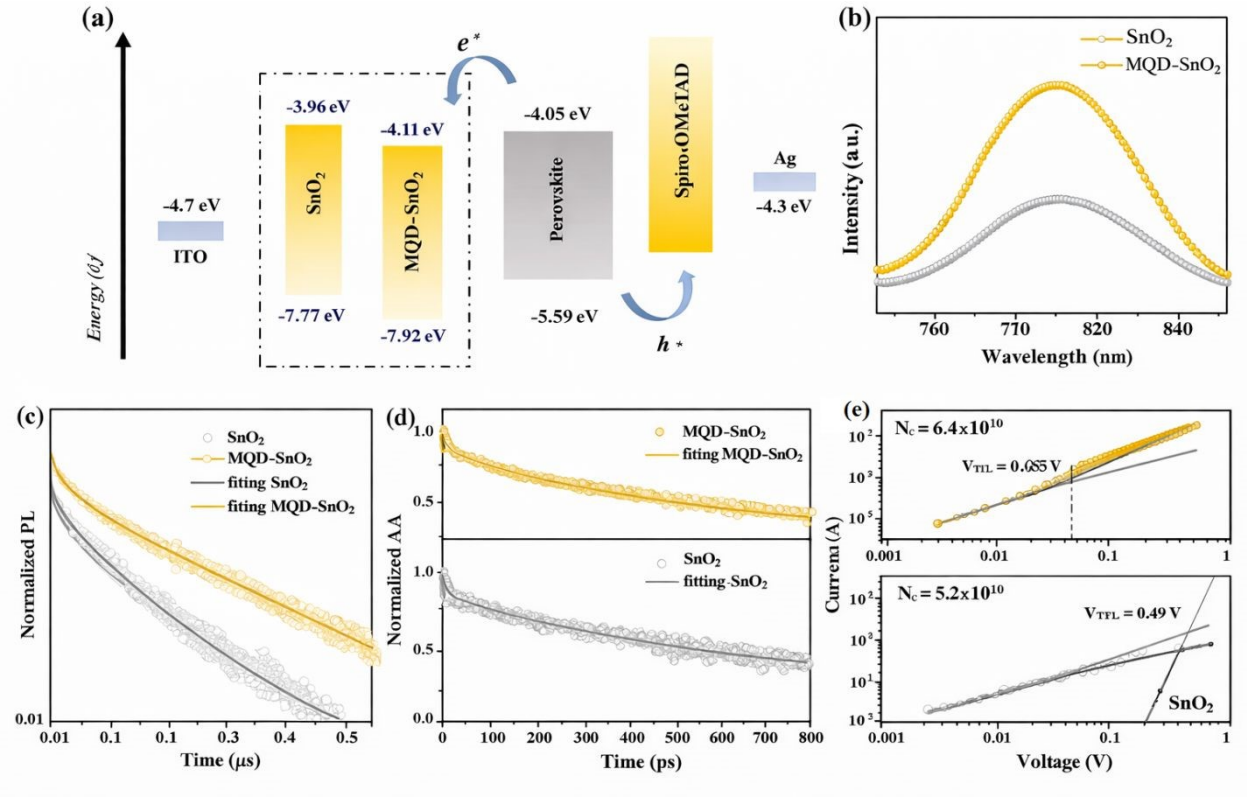

Figure 4. Charge dynamics in MQD-modified SnO_2 ETLs. (a) Energy band diagram with improved alignment at MQD-SnO_2/perovskite interface. (b) Steady-state PL spectra showing intensified emission for MQD-SnO_2 due to reduced nonradiative recombination. (c) TRPL curves with prolonged lifetime. (d) TA decay kinetics indicating faster electron injection. (e) SCLC curves revealing reduced trap density. Adapted with permission from Ref. [80]. © 2023 Elsevier B.V.

Beyond steady-state electrical improvements, MQD-modified ETLs also enable low-temperature processing routes. By combining in-situ oxidized MXene nanoflakes with MQDs, efficient ETLs can be fabricated at temperatures below 100 °C, which is critical for flexible and large-area PSCs [81]. In such systems, MQDs play a decisive role in retarding interfacial recombination and optimizing charge transfer kinetics, demonstrating that MQDs are not merely passive fillers but active electronic regulators within ETLs.

4.2. Regulation of Perovskite Crystallization and Film Quality

Perovskite film quality is a decisive factor governing both efficiency and long-term stability of PSCs. MQDs have demonstrated a unique capability to regulate perovskite crystallization kinetics through strong chemical interactions with precursor species and crystal surfaces. When

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MQDs are introduced at the perovskite/ETL interface or within precursor solutions, they can act as heterogeneous nucleation sites that accelerate initial nucleation while suppressing uncontrolled crystal growth [82]. In situ synchrotron-based grazing-incidence X-ray diffraction measurements reveal that MQD-modified substrates induce the formation of intermediate perovskite phases during anti-solvent treatment, leading to highly crystalline films with improved phase purity and structural stability.

Similarly, MQDs added directly into perovskite precursor solutions can retard crystallization rates through strong interactions between surface terminations (e.g., Cl^-, F^-) and Pb^{2+} ions, promoting preferred grain orientation and reducing residual strain [83]. These effects collectively yield perovskite films with enlarged grains, reduced grain boundary density, and significantly fewer trap states. Importantly, this crystallization control is achieved without compromising film coverage or thickness uniformity, underscoring the compatibility of MQDs with scalable deposition processes.

4.3. Defect Passivation and Suppression of Nonradiative Recombination

Nonradiative recombination at defects and interfaces remains a primary efficiency-limiting factor in PSCs. MQDs exhibit exceptional defect passivation capability due to their rich surface chemistry and strong binding affinity with undercoordinated ions. Experimental evidence consistently demonstrates that MQDs can simultaneously interact with metal cations in charge transport layers (e.g., Sn^{4+} in SnO_2) and Pb^{2+} ions in perovskite films, forming robust chemical bonds that neutralize deep trap states [80]. This bifunctional passivation mechanism is particularly effective at buried interfaces, where defect densities are typically highest and most difficult to access using conventional surface treatments.

Functionalized MQDs further expand this capability. For instance, fluorine-terminated MQDs not only passivate defects but also introduce p-type characteristics that favor hole transfer while suppressing interfacial recombination in inorganic perovskites [84]. As a result, devices exhibit substantially reduced energy losses and near-record open-circuit voltages, highlighting the critical role of MQD surface chemistry in defect regulation.

4.4. Interface-Specific Energy-Level Engineering and Charge Extraction

Beyond defect passivation, MQDs play a decisive role in engineering energy-level alignment at critical interfaces within PSCs. By virtue of their tunable electronic structure and surface dipoles, MQDs enable precise modulation of interfacial band offsets, facilitating directional charge extraction. At the perovskite/ETL interface, MQDs reduce electron extraction barriers and suppress back-transfer by optimizing conduction band alignment [82]. Conversely, MQDs can also be tailored for hole-selective interfaces. In wide-bandgap and inverted PSCs, MQD-engineered NiO_x HTLs exhibit improved conductivity, enhanced surface hydroxylation, and superior energy alignment with perovskite absorbers, enabling highly efficient charge extraction [86].

The effectiveness of MQDs as interfacial energy modifiers is further amplified when dual-interface strategies are employed. Simultaneous MQD-based engineering at both electron- and

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hole-selective interfaces leads to synergistic improvements in carrier extraction efficiency, hysteresis suppression, and fill factor enhancement [86]. These results underscore the adaptability of MQDs across different interface types and device architectures.

Figure 5 summarizes the impact of MQD incorporation into the SnO_2 electron transport layer on the performance of planar perovskite solar cells with the ITO/SnO_2 (or MQD-modified SnO_2)/perovskite/Spiro-OMeTAD/MoO_3/Au configuration. As shown in panel (A), MQDs enable interfacial energy-level engineering by tuning the electronic structure and surface dipoles of SnO_2, thereby improving conduction-band alignment at the perovskite/ETL interface and facilitating electron extraction while suppressing charge back-transfer. Consistent with this effect, panel (B) shows that the MQD-modified device exhibits higher photovoltaic performance than the pristine SnO_2-based reference, achieving a PCE of 23.34% with improved V_{OC}, J_{SC}, and FF, together with negligible hysteresis. The stabilized power output in panel © further confirms the reliability of the improved performance, with the target device maintaining ~23% efficiency under steady-state operation. Panel (D) presents enhanced IPCE over the visible range, indicating more efficient charge collection and reduced interfacial recombination. In addition to performance enhancement, panels (E) and (F) demonstrate that MQD-based interface engineering also improves device stability under continuous illumination and ambient storage. These results collectively show that MQDs function as effective interfacial modifiers that simultaneously optimize energy-level alignment, promote balanced charge transport, reduce nonradiative losses, and improve the operational durability of perovskite solar cells.

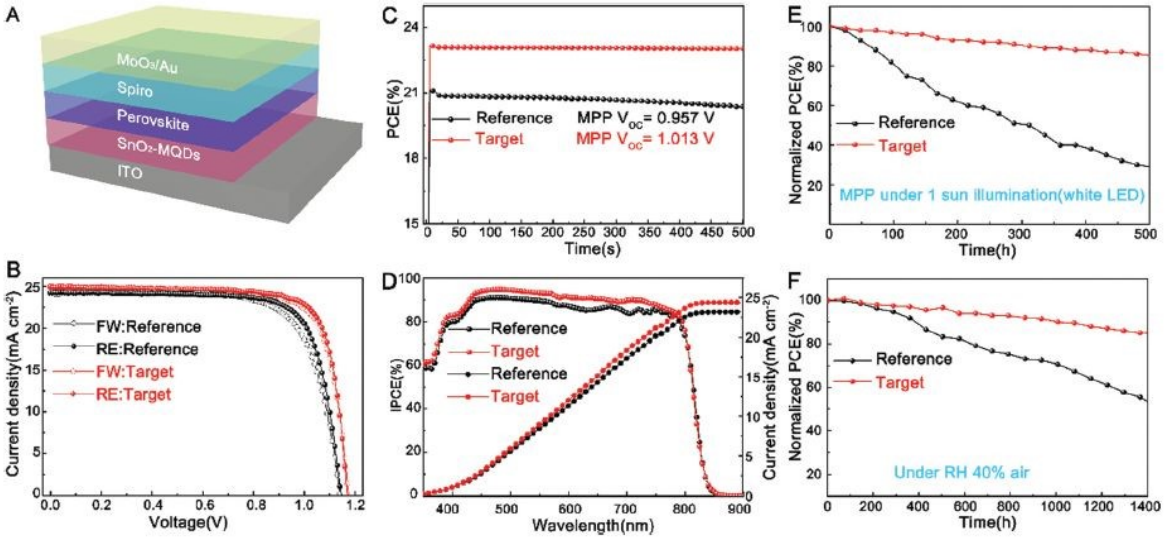

Figure 5. Performance of MQD-SnO_2-based PSCs. (A) Device structure. (B) J–V curves with PCEs of 20.96% (reference) and 23.34% (target), minimal hysteresis. (C) Stabilized PCE. (D) IPCE with integrated J_{sc} ~24.39 mA cm^{-2} (target). (E) Light-soaking stability. (F) Ambient stability (40–60% RH, ~90% retention after 1400 h). Adapted with permission from Ref. [82]. © 2021 Royal Society of Chemistry

4.5. Stability Enhancement under Environmental and Thermal Stress

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Long-term stability remains a major bottleneck for PSC commercialization. MQDs contribute to stability enhancement through multiple complementary mechanisms, including defect passivation, barrier formation against moisture ingress, and suppression of interfacial chemical reactions. Devices incorporating MQD-modified ETLs exhibit remarkable ambient stability, retaining over 95% of their initial efficiency after more than 1000 hours of storage under moderate humidity conditions [80]. Similarly, MQD-treated perovskite films show significantly improved resistance to moisture-induced degradation due to the formation of hydrophobic and chemically robust interfacial networks [83].

Thermal stability is also substantially enhanced. MQD-based interfaces maintain structural and electronic integrity under prolonged heating at elevated temperatures, outperforming conventional oxide-based interfaces [85]. These stability improvements are not merely secondary effects but are directly linked to reduced defect densities, suppressed ion migration, and stabilized interfacial bonding configurations.

4.6. Architecture-Dependent Applications and Advanced Device Configurations

The versatility of MQDs is further demonstrated by their successful integration into diverse PSC architectures, including regular (n–i–p), inverted (p–i–n), flexible, and tandem configurations. In flexible PSCs, MQDs enable low-temperature processing of efficient ETLs, addressing a critical limitation of traditional oxide layers [81]. In inverted architectures, MQD-engineered NiO_x HTLs support high-efficiency wide-bandgap perovskites, facilitating their integration into tandem devices [85]. Moreover, the combined use of zero-dimensional MQDs and two-dimensional MXene nanosheets allows complementary regulation of perovskite bulk and transport layer properties, leading to synergistic performance enhancements. This dimensional hybridization strategy highlights the broader design space enabled by MXene-based materials. In tandem solar cells, MQD-engineered transport layers enable record-level efficiencies by ensuring optimal energy alignment, reduced recombination losses, and enhanced interfacial stability [85]. These achievements demonstrate that MQDs are not limited to laboratory-scale PSCs but are compatible with advanced photovoltaic technologies targeting practical deployment.

4.7. Mechanistic Insights into MQD-Enhanced PSC Performance

The performance improvements observed in PSCs incorporating MQDs arise from a combination of interrelated physical and chemical mechanisms that operate at multiple hierarchical levels, including charge transport layers, perovskite bulk, and buried interfaces. One primary mechanism is defect passivation. MQDs, with their rich surface terminations (–O, –OH, –F, –Cl), form strong chemical interactions with undercoordinated Pb^{2+} ions in perovskite grains and Sn^{4+} or Ni^{3+} in ETL and HTL layers, effectively neutralizing deep trap states and suppressing nonradiative recombination [80, 84]. This dual interfacial passivation is central to the observed reduction in defect density and corresponding increases in open-circuit voltage (V_{OC}) and fill factor.

A second mechanism involves energy-level modulation and band alignment optimization. The intrinsic dipoles of MQDs induce local vacuum-level shifts at the ETL/perovskite and

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HTL/perovskite interfaces, thereby facilitating directional charge extraction and reducing interfacial barriers [82, 85]. Fluorine- or chlorine-terminated MQDs further adjust the valence and conduction bands to create favorable offsets for electron and hole transport, minimizing recombination losses and enabling hysteresis-free operation. This effect is especially pronounced when MQDs are strategically positioned at both electron- and hole-selective interfaces [86]. MQDs also modulate perovskite crystallization kinetics, serving as heterogeneous nucleation centers that control the growth rate, grain orientation, and phase stability of perovskite films [83]. By retarding uncontrolled crystallization and promoting uniform intermediate-phase formation during anti-solvent treatment, MQDs lead to enlarged grains, reduced grain boundaries, and lower residual strain. Such microstructural improvements directly enhance carrier mobility and device stability.

Finally, MQDs act as multifunctional charge transport facilitators. Their zero-dimensional structure allows localized electronic coupling without compromising film continuity, providing intermediate energy states that enhance interfacial charge transfer. Additionally, MQDs contribute to environmental resilience by forming hydrophobic barriers and stabilizing interfacial networks against moisture, light, and thermal stress, which is critical for long-term operational stability [85].

Table 2 summarizes the main integration strategies of MQDs in PSCs and correlates their interfacial functions with device-level performance improvements. Across different device configurations, MQDs act as multifunctional interfacial modifiers by simultaneously facilitating defect passivation, tuning energy-level alignment, regulating perovskite crystallization, and promoting charge extraction. In electron- and hole-transport layers, MQDs can improve conductivity, suppress trap-assisted recombination, and optimize carrier selectivity. When introduced at critical interfaces or into precursor formulations, they also contribute to improved film morphology, reduced nonradiative losses, and enhanced environmental stability. These effects operate synergistically, explaining why MQD incorporation often leads to higher power conversion efficiency, suppressed hysteresis, and improved operational durability across a wide range of PSC architectures, including low-temperature and tandem devices.

Table 2. Representative application strategies of MQDs in PSCs and their effects on device performance

MQD integration location	MQD type / surface chemistry	Primary functions	Key effects on perovskite or transport layers	Main device improvements	Ref.
SnO_2 ETL (hybrid MQDs–SnO_2)	$Ti_3C_2T_x$ MQDs (–O, –OH, –F)	Increased ETL conductivity; reduced SnO_2 defects; optimized band alignment; dual defect passivation	Improved perovskite film quality; reduced interfacial recombination; enhanced charge transport	PCE: 17.44% → 21.63%; defect density: 5.21×10^{21} → 6.4×10^{20} cm^{-3}; ~96% PCE retention after 1128 h	[80]
Perovskite/TiO_2 ETL interface + HTL	$Ti_3C_2T_x$ MQDs + $Cu_{1.8}S$ NCs	Dual-interface engineering; enhanced electron/hole extraction; improved	Larger grain size; suppressed hysteresis; faster carrier extraction	PCE: 18.31% → 21.64%; hysteresis-free behavior; improved light	[86]

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		crystallinity		stability	
SnO_2 ETL (MQD-modified)	$Ti_3C_2T_x$ MQDs	Regulation of perovskite nucleation; intermediate-phase formation; improved charge extraction	Highly crystalline and phase-stable perovskite films	Steady-state PCE up to 23.3%; excellent humidity and light-soaking stability	[82]
NiO_x HTL (MQD-engineered)	$Ti_3C_2T_x$ MQDs (–OH, –O, –F)	Improved conductivity; surface hydroxylation; enhanced SAM anchoring; energy-level alignment	Reduced interfacial defects; improved wide-bandgap perovskite crystallinity	Opaque PSC PCE: 22.96%; tandem efficiency: 31.06% (2T), 32.20% (4T)	[85]
Low-temperature ETL (≤100 °C)	In situ oxidized MXene + MQDs	Bandgap opening of metallic MXene; MQD-assisted band alignment; reduced recombination	Improved perovskite film quality; enhanced charge transfer	PCE: 7.42% → 20.16%; highest reported efficiency among ETLs processed at ≤100 °C	[81]
Interface passivation (inorganic PSCs)	F-terminated $Ti_3C_2F_x$ MQDs	Energy-level tuning; facilitated hole transfer; moisture-barrier formation	Reduced nonradiative recombination; improved interface stability	$CsPbI_3$ PSC PCE: 20.44%; V_{OC} = 1.22 V; 93% retention after 600 h	[84]
Perovskite precursor additive	Cl-terminated $Ti_3C_2Cl_x$ MQDs	Retarded crystallization; preferred orientation; strain relaxation	Higher crystallinity; fewer trap states; improved band alignment	PCE: 21.31%; V_{OC} = 1.19 V; >84% PCE retention after 1000 h at 40% RH	[83]

4.8. Critical Perspective on the Practical Limitations and Unresolved Issues of MQD-Based Strategies

Although the integration of MQDs into PSCs has produced encouraging improvements in photovoltaic performance, the currently available evidence also reveals several practical limitations and unresolved issues that must be critically considered. A major concern is that the beneficial effects of MQDs are highly context-dependent and cannot yet be regarded as universally reproducible across different device architectures and processing routes [80–82]. In many reports, performance enhancement is attributed to improved conductivity, better energy-level alignment, or defect passivation; however, these effects are often discussed independently, even though they are strongly interrelated at the device level [81, 84].

Another important issue is the narrow optimization window associated with MQD incorporation. While moderate MQD loading may improve interfacial contact and charge extraction, excessive incorporation can alter film morphology, disturb layer uniformity, or create additional electronic inhomogeneity, thereby offsetting the intended benefits [80, 82]. This suggests that MQDs should not be viewed simply as universally beneficial additives, but rather as highly sensitive functional modifiers whose effects depend on concentration, dispersion quality, and interfacial compatibility.

The literature also indicates that the mechanistic interpretation of MQD function is not always sufficiently rigorous. For example, improved device efficiency is frequently correlated with

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reduced recombination or enhanced crystallization, but direct causal separation of these contributions is often lacking [81, 83]. In several cases, multiple mechanisms are proposed simultaneously, including nucleation control, trap passivation, band-edge tuning, and faster carrier extraction, without clearly identifying which effect is dominant under a given set of fabrication conditions [82, 84]. As a result, the field still lacks a unified framework for understanding structure–property–performance relationships in MQD-modified PSCs.

In addition, long-term relevance remains insufficiently validated. Although MQDs are often presented as beneficial for environmental and operational stability, current evidence is still based mainly on laboratory-scale measurements under limited testing conditions [83]. Comparisons across studies remain difficult because aging protocols, humidity control, illumination intensity, and encapsulation conditions are not fully standardized [82, 86]. Therefore, the true contribution of MQDs to durable device operation cannot yet be assessed with high confidence.

Taken together, these observations indicate that the future progress of MQD-based PSCs will depend not only on demonstrating higher efficiency, but also on establishing reproducible processing windows, clarifying dominant working mechanisms, and adopting more standardized stability evaluation protocols [84,86]. Such critical assessment is essential for translating promising laboratory results into credible technological advancement.

4.9. Integrated Overview of MQD-Based Strategies and Their Remaining Limitations

The studies discussed in this section collectively demonstrate that MQDs can improve the performance of perovskite solar cells through several complementary mechanisms. These strategies mainly include the incorporation of MQDs into charge-transport layers, modulation of perovskite crystallization processes, defect passivation within the perovskite lattice, and interfacial energy-level engineering. When integrated into electron-transport layers, MQDs can enhance electrical conductivity and facilitate more efficient electron extraction, thereby reducing charge recombination losses. In parallel, their presence during perovskite film formation can influence nucleation and crystal growth behavior, often leading to larger grain sizes and improved film uniformity. MQDs have also been shown to passivate undercoordinated ions and surface defects, which reduces trap-assisted recombination [81, 83]. Furthermore, the tunable surface terminations of MQDs enable modification of interfacial electronic structures, which can improve band alignment and carrier transport across device interfaces.

Despite these advantages, several important limitations remain that currently constrain the broader implementation of MQD-based strategies. First, the beneficial effects of MQDs are frequently sensitive to concentration and processing parameters, resulting in relatively narrow optimization windows. Small variations in MQD loading or deposition conditions can significantly alter crystallization dynamics or interfacial energetics, sometimes leading to inconsistent device performance across studies. Second, the mechanisms responsible for performance enhancement are often difficult to isolate, as MQDs may simultaneously influence nucleation behavior, defect passivation, and charge transport. This overlap makes it challenging to determine which mechanism dominates in specific device architectures [82, 85].

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Another limitation concerns the variability in synthesis and surface chemistry of MQDs, which can strongly influence their interaction with perovskite materials and transport layers. Differences in size distribution, functional groups, and surface terminations may lead to different electronic interactions at interfaces, complicating comparisons between studies. Additionally, while many reports demonstrate improvements in device efficiency, long-term operational stability remains insufficiently characterized in several cases, particularly under realistic environmental and illumination conditions [80, 85].

Taken together, these limitations highlight important opportunities for future research. More systematic studies that decouple crystallization, passivation, and interfacial effects are needed to clarify the dominant mechanisms governing MQD-assisted performance improvements. In addition, improved control over MQD synthesis and surface chemistry, combined with standardized stability evaluation protocols, will be essential for translating laboratory-scale demonstrations into more reliable and scalable photovoltaic technologies.

5. Challenges and Future Perspectives

Despite the remarkable advancements in PSCs enabled by MQDs, several critical challenges remain before their full potential can be realized in practical applications. Addressing these issues requires a comprehensive understanding of the interplay between MQD properties, device architecture, and processing conditions. This section highlights the main obstacles, technological bottlenecks, and future directions for the integration of MQDs in PSCs.

5.1. Scalability and Controlled Synthesis of MQDs

A fundamental challenge lies in the scalable production of MQDs with uniform size, surface terminations, and electronic properties. Most experimental studies rely on hydrothermal or etching-assisted methods that produce small batches of MQDs with variable lateral sizes and functional group distributions [80]. Such heterogeneity can lead to inconsistent device performance, as the extent of defect passivation, energy-level alignment, and crystallization control are highly sensitive to MQD surface chemistry. Future efforts should focus on standardized, high-yield synthesis techniques, potentially combining top-down etching with bottom-up assembly to maintain tunable size distributions while preserving functional terminal groups.

5.2. Interface-Specific Integration Challenges

While MQDs exhibit exceptional interfacial functionalities, their incorporation into multi-layer PSC architectures is non-trivial. Poor dispersion or aggregation can create localized charge traps or morphological defects, counteracting their intended effects. Additionally, the optimal concentration and spatial distribution of MQDs are strongly device-dependent. Excessive loading can impede charge transport, whereas insufficient incorporation limits defect passivation and crystallization control [86]. Development of controlled deposition strategies, such as spin-coating with surface-active ligands or layer-by-layer assembly, may overcome these limitations and enable reproducible interface engineering.

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5.3. Stability under Operational and Environmental Stress

Despite demonstrated improvements in moisture and thermal stability, MQD-based PSCs still face long-term operational challenges, especially under combined stress conditions of light, heat, and humidity [83]. The durability of MQD-perovskite interfaces under continuous illumination or thermal cycling has not yet been fully quantified, particularly for tandem or flexible architectures. Future research should target accelerated lifetime testing and mechanistic studies of degradation pathways, including ion migration, interfacial delamination, and chemical interactions with residual solvents or ambient species.

5.4. Compatibility with Diverse Device Architectures

Current studies predominantly explore MQDs in n-i-p planar structures or inverted p-i-n devices, with limited reports on tandem, flexible, or large-area modules [81]. Scaling up to commercially relevant areas requires attention to film uniformity, defect control, and low-temperature processing, particularly for flexible substrates. The integration of MQDs in wide-bandgap perovskites or in top-cell layers for tandem configurations also demands precise energy-level tuning to avoid interfacial recombination and maximize charge extraction efficiency.

5.5. Understanding Mechanistic Complexity

While significant progress has been made in elucidating MQD-mediated performance enhancements, the mechanistic understanding remains incomplete. Interactions between MQDs and perovskite precursors, buried defects, and transport layers involve simultaneous chemical, electronic, and electrostatic effects. Advanced characterization techniques, such as in situ synchrotron X-ray diffraction, ultrafast transient spectroscopy, and high-resolution electron microscopy, are essential to capture real-time crystallization dynamics, interfacial energy shifts, and charge transfer kinetics. Computational modeling, including DFT and molecular dynamics, can complement experimental studies to predict optimal MQD compositions, surface terminations, and distributions.

5.6. Optimizing Multifunctional Roles

MQDs are inherently multifunctional, simultaneously affecting charge transport, crystallization, defect passivation, and environmental stability. However, balancing these effects is non-trivial. For instance, a surface termination that enhances defect passivation may compromise energy-level alignment or charge mobility [84]. Future strategies should aim at tailored MQD design, such as selective functionalization, hybrid 0D/2D MXene integration, or gradient distribution across the ETL and perovskite layers, to maximize synergistic benefits.

5.7. Integration with Low-Temperature and Flexible Processing

The low-temperature processability of MQDs makes them highly suitable for flexible PSCs and tandem architectures [81]. However, ensuring consistent film formation and interfacial contact at sub-100°C remains challenging. MQDs must facilitate not only charge extraction but also

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perovskite nucleation under constrained thermal budgets. Future work should explore combinatorial approaches, such as in situ oxidation, surface ligand engineering, and co-deposition with metal oxide nanoparticles, to achieve robust low-temperature interfaces.

5.8. Prospects for Commercialization

For MQD-enabled PSCs to reach commercialization, several criteria must be simultaneously met: high efficiency (>25%), long-term operational stability, low-cost scalable synthesis, and compatibility with module fabrication. The multifunctionality of MQDs offers a unique opportunity to address multiple bottlenecks in a single additive; however, systematic optimization and standardization are required. The development of design rules linking MQD physicochemical properties to device performance metrics will be essential to translate lab-scale success to industrial application.

5.9. Future Research Directions

Although significant progress has been achieved in integrating MQDs into perovskite solar cells, several research directions remain critical for advancing this field toward practical applications. One important priority is the development of high-throughput and controllable synthesis methods capable of producing MQDs with precisely defined size distributions, surface terminations, and functional groups. Such control is essential because the optoelectronic properties of MQDs and their interactions with perovskite materials are strongly influenced by these parameters.

Another important direction involves deeper mechanistic understanding of how MQDs influence device performance. Future studies combining in situ or operando characterization techniques—such as time-resolved spectroscopy, synchrotron-based measurements, and advanced microscopy—with computational modeling can help clarify the mechanisms governing defect passivation, band alignment, and crystallization dynamics [80, 84]. These approaches would enable researchers to distinguish between the multiple roles that MQDs may simultaneously play in photovoltaic devices.

Scalable device fabrication is also an essential challenge. While many studies demonstrate promising performance improvements at laboratory scale, translating these results to large-area, flexible, or tandem perovskite devices requires deposition strategies that ensure uniform MQD distribution and reproducible interface engineering. Techniques compatible with industrial processing will therefore be important for future development.

Long-term operational stability represents another key research priority. Systematic stability investigations under realistic working conditions—including continuous illumination, thermal stress, humidity exposure, and electrical bias—are necessary to evaluate the durability of MQD-

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modified devices. Accelerated aging tests and standardized stability protocols would help establish meaningful comparisons between different studies [83].

Finally, emerging hybrid architectures that combine zero-dimensional MQDs with two-dimensional MXene nanosheets may provide new opportunities to exploit synergistic effects in charge transport, defect passivation, and interface stabilization. Collectively, these research directions highlight that the integration of MQDs into perovskite solar cells remains a multidisciplinary challenge requiring coordinated advances in materials chemistry, device engineering, and theoretical modeling [81].

6. Conclusions

MQDs have emerged as a highly versatile and multifunctional class of nanomaterials with profound impacts on PSC performance. Their zero-dimensional structure, tunable surface chemistry, and unique electronic properties enable them to act simultaneously as defect passivators, interfacial energy-level modulators, crystallization directors, and charge transport facilitators. Through strategic incorporation into ETLs, HTLs, perovskite precursor solutions, or interfacial regions, MQDs enhance power conversion efficiency (PCE), reduce hysteresis, and improve operational stability across diverse PSC architectures, including planar, inverted, flexible, wide-bandgap, and tandem devices. Mechanistically, MQDs reduce defect densities by forming strong chemical interactions with undercoordinated ions, induce favorable band alignment via surface dipoles, guide nucleation and growth to produce highly crystalline and uniform perovskite films, and facilitate localized charge transfer through intermediate electronic states. These synergistic effects collectively contribute to both enhanced photovoltaic performance and prolonged device longevity, demonstrating that even nanoscale additives can exert a disproportionate influence on PSC efficiency and stability.

Despite these advances, several challenges remain. Achieving scalable, reproducible, and compositionally controlled MQDs, ensuring uniform integration across large-area devices, and understanding the complex interplay between multifunctional roles and device-specific architectures are critical for the commercialization of MQD-based PSCs. Furthermore, systematic mechanistic studies, long-term operational stability testing, and low-temperature processing strategies must be pursued to fully leverage the potential of MQDs in flexible and tandem solar cell technologies. Looking forward, the combination of advanced synthetic control, in situ characterization, computational modeling, and device engineering will be pivotal to optimize MQD properties and their integration strategies. Addressing these challenges promises not only to unlock higher efficiencies and stability in PSCs but also to broaden the applicability of MQDs to other optoelectronic devices, including photodetectors, light-emitting diodes, and tandem photovoltaic systems. Collectively, these insights establish MQDs as a key enabling material for the next generation of high-performance, durable, and scalable PSCs.

Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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This article is a review and does not include any new experimental data. All data discussed and analyzed are derived from previously published studies, which are appropriately cited in the manuscript. No new datasets were generated or analyzed during the current study.