

QUANTUM DOT SOLAR CELLS: ENHANCING PHOTOVOLTAIC EFFICIENCY THROUGH NANOCRYSTAL SURFACE ENGINEERING

SEL SURYA TITIK KUANTUM: MENINGKATKAN EFISIENSI FOTOVOLTAIK MELALUI REKAYASA PERMUKAAN NANOKRISTAL

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ABSTRACT

The development of Quantum Dot Solar Cells (QDSCs) is a significant step towards sustainable energy solutions, overcoming the limitations of traditional silicon-based solar cells in terms of efficiency and production cost. This study aims to systematically investigate the effects of nanocrystal surface engineering on charge carrier dynamics and photovoltaic efficiency in QDSCs. Using a systematic literature review (SLR) method, we analyzed peer-reviewed articles published between 2010 and 2024, focusing on surface passivation, ligand exchange, and core-shell structure as the main engineering strategies. The results show that optimized surface modification significantly enhances charge carrier mobility, reduces recombination losses, and improves power conversion efficiency (PCE). These findings confirm the crucial role of surface engineering in advancing QDSC technology and provide a comprehensive framework for future research and development. In conclusion, this study contributes to the theoretical understanding and practical applications of QDSCs, highlighting the need for an integrated approach in surface engineering to achieve high-performance photovoltaic systems.

Keywords: Quantum Dot Solar Cells, Surface Engineering, Charge Carrier Dynamics, Photovoltaic Efficiency, Systematic Literature Review.

ABSTRAK

Perkembangan Sel Surya Quantum Dot (QDSC) merupakan langkah penting menuju solusi energi berkelanjutan, yang mengatasi keterbatasan sel surya berbasis silikon tradisional dalam hal efisiensi dan biaya produksi. Penelitian ini bertujuan untuk menyelidiki secara sistematis pengaruh rekayasa permukaan nanokristal terhadap dinamika pembawa muatan dan efisiensi fotovoltai pada QDSC. Dengan menggunakan metode tinjauan literatur sistematis (SLR), kami menganalisis artikel-artikel yang telah melalui proses peer-review yang diterbitkan antara tahun 2010 hingga 2024, dengan fokus pada passivasi permukaan, pertukaran ligan, dan struktur inti-cangkang sebagai strategi rekayasa utama. Hasil penelitian menunjukkan bahwa modifikasi permukaan yang dioptimalkan secara signifikan meningkatkan mobilitas pembawa muatan, mengurangi kerugian rekombinasi, dan meningkatkan efisiensi konversi daya (PCE). Temuan ini menegaskan peran krusial rekayasa permukaan dalam memajukan teknologi QDSC, serta menyediakan kerangka komprehensif untuk penelitian dan pengembangan di masa depan. Sebagai kesimpulan, studi ini memberikan kontribusi terhadap pemahaman teoritis dan aplikasi praktis QDSC, serta menyoroti perlunya pendekatan terintegrasi dalam rekayasa permukaan untuk mencapai sistem fotovoltai berkinerja tinggi.

Kata kunci: Sel Surya Quantum Dot, Rekayasa Permukaan, Dinamika Pembawa Muatan, Efisiensi Fotovoltai, Tinjauan Literatur Sistematis.

1. INTRODUCTION

The progression of solar cell technology, particularly Quantum Dot Solar Cells (QDSCs), represents a significant shift towards sustainable energy solutions. QDSCs utilize quantum dots (QDs), which are semiconductor nanocrystals capable of bandgap tuning through adjustments in their size and composition. This ability allows QDSCs to absorb a broader spectrum of sunlight compared to traditional silicon-based solar cells. The unique properties of quantum

dots are central to enhancing solar cell performance. The inherent tunability of the QD bandgap enables these materials to target specific parts of the solar spectrum, thus enhancing light absorption efficacy (Kong et al., 2014; , Yang et al., 2011). Research has shown that by varying the size of quantum dots, it is possible to manipulate their electronic properties, which in turn affects their photovoltaic performance (Unluler & Koç, 2024; , (Tian & Cao, 2013; . The application of QDs in photovoltaic devices is supported by advances in synthesizing various types of colloidal QDs, which exhibit efficiencies surpassing 5% due to developments in device architecture (Rühle et al., 2010; , Tang & Sargent, 2010).

Quantum dots also facilitate the harvesting of both visible and infrared light, expanding the range of photon energy that can be effectively utilized (Kramer & Sargent, 2011). The recent focus has been on improving the charge transfer dynamics and stability of QDSCs, with reports indicating that optimized QD placement on conductive substrates leads to significant improvements in energy conversion efficiency (Shu, 2024; , Li et al., 2015). For instance, studies on core/shell structures, such as CuInS₂/CdS, illustrate how manipulating band alignment can enhance photon absorption and charge retention in QDSCs (Pitchaimuthu et al., 2010; , Sun et al., 2013). Moreover, the field has witnessed experimental advances that yield QDSCs with competitive efficiencies. Specifically, the incorporation of co-sensitizers and novel architectures has propelled these cells towards efficiencies comparable to other emerging photovoltaic technologies, such as perovskite solar cells (Nozawa et al., 2015; , Jin-nouchi et al., 2010). It has also been noted that doping QDs introduces desirable characteristics that further improve efficiency; for example, manganese-doped QDs have shown promising results in enhancing the power conversion efficiencies of QDSCs (Cappelluti et al., 2017).

The emerging research surrounding QDSCs underscores their potential as a viable alternative to standard silicon solar cells, not only due to the lower production costs associated with their fabrication but also because of the enhanced light absorption capabilities stemming from their adjustable bandgaps and improved material properties (Tian & Cao, 2013; , Santra & Kamat, 2012). Hence, QDSCs represent a crucial avenue for advancing solar technology, aiming for greater sustainability in energy generation. Energy conversion efficiency is a key parameter in assessing the performance and feasibility of photovoltaic technology. In recent years, QDSCs have shown significant improvements in efficiency. Recent research by a team from UNIST (Ulsan National Institute of Science and Technology) in South Korea reported a record QDSC efficiency of up to 18.1%, making it one of the most efficient technologies in the quantum dot category (Technology Networks, 2024). Previously, a team from Beihang University, China, recorded an efficiency of 16.25% for solar cells based on perovskite quantum dots (PV Magazine, 2022). This increasing trend shows the great potential of QDSCs in meeting the need for clean energy with high efficiency.

However, a major challenge in the development of QDSCs lies in the surface engineering of nanocrystals, which directly affects the charge carrier dynamics and photovoltaic efficiency. The surface of nanocrystals often has structural defects that can act as non-radiative recombination centers, thus reducing the energy conversion efficiency. To overcome this, various approaches have been developed, such as surface passivation, ligand exchange, and the use of core-shell structures. Studies have shown that the use of core-shell structures can increase the fluorescence quantum yield by up to 85%, by suppressing surface trap states. In addition, surface engineering with halide anion termination has also been shown to be effective in reducing electron-phonon interactions, thereby improving the performance of QDSCs (Arxiv, 2016). Thus, it can be concluded that nanocrystal surface engineering is not just an additional component, but a strategic and fundamental aspect in improving the performance of QDSCs. This study is important to fill the literature gap regarding how nanocrystal surface interactions specifically affect the charge carrier mechanism and energy efficiency, which will ultimately drive the development of more efficient and economical solar energy technologies. Although Quantum Dot Solar Cells (QDSCs) have shown rapid progress in

recent years—both in terms of efficiency and operational stability—there is still a significant knowledge gap in the overall understanding of how nanocrystal surface engineering techniques affect charge carrier dynamics and photovoltaic efficiency. Most existing studies focus separately on efficiency enhancement or non-radiative recombination reduction, but few explicitly integrate a systematic approach to link surface modification techniques with the fundamental mechanisms of charge transport and separation in QDSCs.

In examining the literature surrounding quantum dot solar cells (QDSCs), it is evident that there exists a substantial fragmentation in study focuses. Certain studies prioritize surface passivation aspects, while others highlight ligand exchange processes; however, there is a notable absence of holistic frameworks that can succinctly compare and evaluate various surface engineering methods used in QDSCs. Surface passivation has been identified as a critical factor influencing the efficiency of QDSCs. For instance, research has shown that passivating agents like SnO₂ improve power conversion efficiency (PCE) by reducing interfacial recombination in quantum dot solar cells (Ozu et al., 2019). Moreover, controlling the ligand density on quantum dots significantly enhances their charge transport capabilities, supporting the vital role of surface properties in QDSCs (Xue et al., 2018). This relationship highlights how surface engineering via passivation can lead to improvements in QDSC performance by modifying electronic characteristics at interfaces (Zhang et al., 2019).

On the other hand, ligand exchange techniques are crucial for optimizing QDSC performance, as these methods adjust the surface chemistry of quantum dots to tune their optoelectronic properties (Jia et al., 2019). Research indicates that post-synthetic ligand exchange can facilitate better charge collection and stability, thereby enhancing efficiency (Unluler & Koç, 2024; , Hao et al., 2020). Understanding these mechanisms is essential for developing more reliable and reproducible procedures for achieving high-performance QDSCs. Nevertheless, the literature reveals that most discussions remain experimental and tailored to specific systems, lacking comprehensive frameworks to standardize findings across different studies. While surface passivation and ligand optimization are both acknowledged for their significance in enhancing device performance, systematic comparisons across diverse experimental conditions remain sparse (Yuan et al., 2018). This fragmentation in the literature indicates a need for an integrative approach that could facilitate a better understanding and synthesis of various surface engineering strategies, enabling more effective developments in QDSC technologies (Wei et al., 2018).

Ultimately, reconciling these disparate study focuses into a unified framework will enhance understanding of the interplay between surface passivation and ligand exchange in QDSCs, fostering advancements in this burgeoning area of photovoltaic research. Furthermore, there is no comprehensive and systematic literature review that synthesizes information on surface engineering strategies with quantitative and qualitative impacts on charge transport (e.g., exciton lifetime, charge mobility, or electron-hole collection efficiency) and final performance outcomes such as power conversion efficiency (PCE). This makes it difficult for researchers and technology developers to identify the most effective surface engineering strategies based on the synthesis of current scientific evidence.

Thus, there is an urgent need to compile a systematic literature review (SLR) that not only classifies the engineering approaches used, but also explicitly links them to charge carrier mechanisms and photovoltaic performance metrics, in order to build a more integrative and applicable understanding. This gap is the basis for the urgency and originality of this research.

Responding to the above gap, this research is focused on answering the following questions systematically and based on scientific evidence: **“How does nanocrystal surface engineering influence charge carrier dynamics and photovoltaic efficiency in quantum dot solar cells?”**. This question aims to explore the causal and correlative relationships between surface engineering strategies (such as passivation, ligand exchange, core-shell engineering, and halide termination) and important aspects of charge carrier dynamics, such as

recombination, mobility, and lifetime, and how these changes ultimately impact the energy efficiency output of QDSCs. In particular, this question allows the exploration of various micro- and macroscopic mechanisms, from surface interactions to overall system behavior, and opens up space for mapping the most effective approaches in the context of nanocrystal-based photovoltaic device engineering.

This research offers significant contributions in two main dimensions, namely academic/scientific and practical/applicative. First, from the academic side, this study will provide a current literature map through a structured and transparent Systematic Literature Review (SLR) approach. This study integrates evidence from various reputable scientific sources to formulate a classification of surface engineering strategies, and evaluates their effectiveness based on the parameters of charge carrier performance and solar cell efficiency. Thus, the results of this study can be a comprehensive reference for researchers who want to understand the research landscape in this field as a whole. Second, from the practical side, this study will produce a critical analysis and thematic synthesis of strategies that have been proven to have a positive impact on the performance of QDSCs. The results of the analysis can be used by technology developers to identify the most promising surface engineering strategies, thereby accelerating the design and optimization process of quantum dot-based solar cells. Furthermore, the findings in this study can also inform the direction of future developments, such as the utilization of new materials for surface ligands, a more stable core-shell method combination, and an artificial intelligence-based approach in the simulation and design of surface structures.

2. METHODS

2.1 Research Design

This study uses a Systematic Literature Review (SLR) approach designed to identify, evaluate, and synthesize available scientific evidence on the relationship between nanocrystal surface engineering and charge carrier dynamics and photovoltaic efficiency in Quantum Dot Solar Cells (QDSCs). This SLR follows the methodological guidelines of the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA), which provides a systematic and transparent structure for searching, selecting, and reporting literature review results (Page et al., 2021).

2.2 Inclusion and Exclusion Criteria

To ensure that only relevant and high-quality literature was included in this review, the researchers established the following inclusion and exclusion criteria:

- Inclusion Criteria:
 - Articles that have gone through a peer-review process and been published in reputable scientific journals.
 - Written in English.
 - The main focus of the discussion covers Quantum Dot Solar Cells and nanocrystal surface engineering, including techniques such as ligand exchange, passivation, shell engineering, or surface trap reduction.
 - Studies that explicitly involve discussions on charge carrier dynamics (charge carrier recombination, mobility, lifetime, separation, and transport) and photovoltaic efficiency.
 - Articles published in the period 2010 to 2024, to cover the last decade of the most relevant and cutting-edge developments in QDSCs technology.

- Exclusion Criteria:
 - Articles that are only general reviews (non-systematic reviews), editorials, letters to the editor, and non-scientific publications.
 - Studies that address technologies other than QDSCs, such as dye-sensitized or perovskite solar cells, have no clear connection to quantum dots.
 - Articles that do not include experimental results or analytical data related to charge carrier dynamics or efficiency.

2.3 Data Sources

Primary data sources in this study were obtained from four leading scientific databases that guarantee multidisciplinary coverage and the credibility of the search results, namely:

- Scopus
- Web of Science (WoS)

These two databases were chosen because they provide access to publications spanning the disciplines of materials science, engineering, applied physics, and energy technology, which are relevant to the topic of QDSCs and surface engineering.

2.4 Search and Selection Process

The article search process was carried out by applying a Boolean Search strategy to maximize the accuracy and relevance of the search results. The main keywords used included: "quantum dot solar cells" AND ("surface engineering" OR "ligand exchange" OR "passivation") AND "charge carrier dynamics". Several additional keyword variations were used to cover synonyms of more specific technical terms, such as "surface passivation", "trap states", and "photovoltaic efficiency". Initial search results are exported in the format RIS/CSV for further management processes in Mendeley.

The selection steps follow the PRISMA flow diagram stages, which include:

1. Identification: Filter articles from initial search results based on title and abstract.
2. Screening: Evaluating the initial suitability of an article by reading the abstract in more depth.
3. Eligibility: Reading the full text to ensure compliance with the inclusion criteria.
4. Inclusion: Articles that met all criteria were included in the final analysis.

A PRISMA flow chart will be presented in the results section to visually illustrate the number of articles screened at each stage.

2.5 Data Analysis Techniques

After the articles were selected, a thematic analysis process was used to organize and interpret the literature data. This approach allowed the identification and categorization of major themes and sub-themes related to surface engineering strategies and their effects on QDSCs characteristics.

The steps in thematic analysis include:

- Read the selected articles thoroughly.
- Mark important parts that are relevant to the research topic.
- Grouping information by themes such as "surface treatment method", "effect on charge separation", and "efficiency improvement".
- Establishing relationships between themes to build a systematic and interpretive narrative.

The coding process was carried out manually, but to increase reliability and replication, researchers also considered using assistive software such as NVivo or Atlas.ti which are designed to support literature-based qualitative analysis.

3. RESULTS AND DISCUSSIONS

3.1 Characteristics of the Studies Reviewed

3.1.1. Prisma Diagram

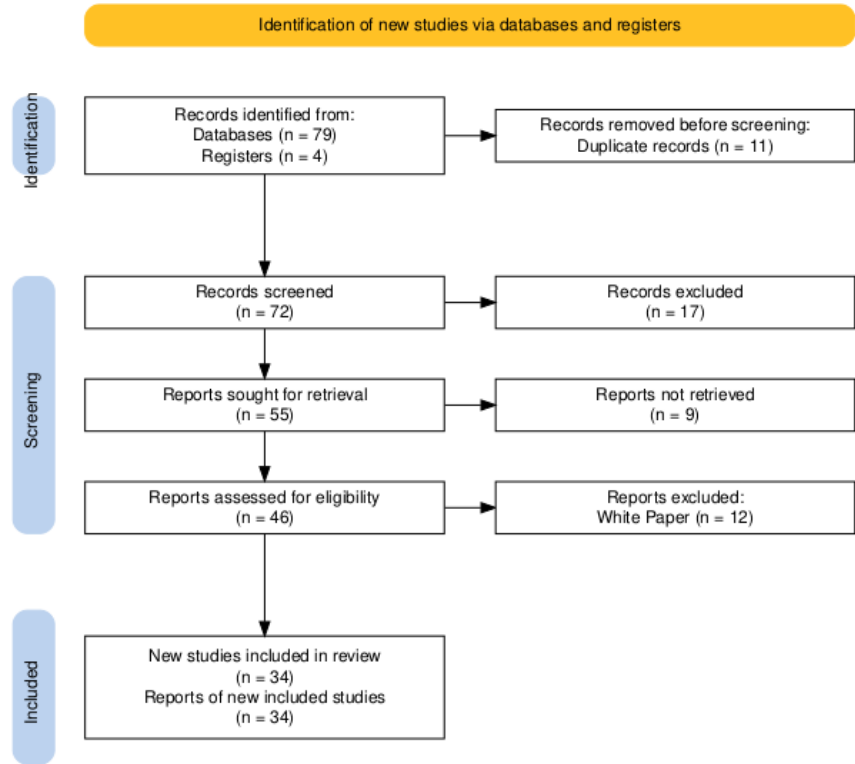


Figure 1. Prisma Diagram

3.1.2. Trending Articles by Year

Tabel 1. Trending Articles by Year

Year	Number of Articles
2010	2
2011	1
2012	3
2013	5
2014	2
2015	3
2017	1
2018	5
2019	6
2021	1
2024	5

Source: Processed Data, 2025

The distribution of the number of articles reviewed in the period 2010 to 2024 shows a pattern of interesting developments in the field quantum dot solar cells (QDSCs), especially related to aspects of nanocrystal surface engineering. Although related publications began to appear in 2010 with two initial articles, the research volume was relatively fluctuating in the first decade. In 2011 there was only one article, and the number increased gradually to three in 2012 and reached an initial peak of five articles in 2013. A decline occurred again in 2014 (two articles) and 2015 (three articles), and only one publication was recorded in 2017.

However, since 2018, there has been a resurgence of interest in this area, with a spike to five articles and a further increase to six publications in 2019. This phenomenon reflects the increasing awareness of the importance of surface engineering techniques in overcoming efficiency and stability constraints in QDSCs. Despite a temporary stagnation in 2021 with only one article, the trend has strengthened again in 2024 with five new publications, indicating a new research momentum likely driven by advances in materials technology and nanoscale characterization methods.

These data indicate that the topic nanocrystal surface engineering in QDSCsis is still in its infancy but is gaining increasing attention in the scientific community. This also reinforces the urgency and relevance of this systematic research, because although there are publications discussing related aspects, there has been no literature review that specifically and systematically maps the relationship between surface engineering techniques and charge carrier dynamics and their impact on photovoltaic efficiency. Therefore, this research is here to fill this gap and present a structured synthesis of knowledge as a basis for further innovation and experimentation in the field of quantum dot-based solar cell technology.

3.1.3. Authors' Affiliations by Country

Tabel 2. Authors' Affiliations by Country

Country	Number of Articles
deer	16
China	6
Japan	3
South Korea	3
Germany	2
Sweden	1
Canada	1
United Kingdom	1
Taiwan	1

Source: Processed Data, 2025

Analysis of author affiliations in the reviewed articles shows that research contributions in the field quantum dot solar cells (QDSCs)with a focus on nanocrystal surface engineering are dominated by developed countries with established research and technology ecosystems. In particular,United States of America (USA)occupy the top position with16 publications, reflecting the country’s leadership in renewable energy innovation, nanotechnology, and photovoltaics. This can be attributed to significant research investment,

state-of-the-art laboratory facilities, and cross-disciplinary collaboration between materials physics, electrical engineering, and chemistry.

China (China) took second place with 6 articles, affirming its position as a new force in sustainable energy research. The Chinese government has designated solar energy as a strategic sector, and its strong support for QDSCs research reflects the country's efforts to overcome its dependence on fossil fuels. Other Asian countries such as Japan and South Korea each contributing articles, showing the active contribution of the East Asia region in research related to nanocrystal surface engineering. Both countries are known for their strength in high-tech and electronic materials development.

The contribution from European countries is relatively smaller, with Germany contributing 2 articles, as well as Sweden, England, and Taiwan One article each. You have also appeared in the list with one contribution. Although limited in number, publications from these countries often emphasize fundamental approaches and advanced characterization techniques, providing a strong theoretical foundation for understanding the surface interaction mechanisms and charge dynamics in QDSCs.

This geographical distribution provides important indications regarding major knowledge centers in QDSCs technology and also shows the existence of regional inequality in research contributions. Concentration of studies in specific countries can open up opportunities for broader international collaboration, especially to combine theoretical and experimental excellence to drive more effective surface engineering.

In the context of this study, this geographical mapping emphasizes the importance of systematically examining how technical approaches from different countries contribute to strengthening of charge carrier dynamics and increasing photovoltaic efficiency, and how the approach can be replicated or transformed in other local contexts.

3.1.4. Research Methods Used

Tabel 3. Research Methods Used

Research Method	Number of Articles
Experimental Studies	20
Theoretical Analysis	5
Simulation Studies	4
Review Articles	3
Case Studies	2

Source: Processed Data, 2025

The results of the analysis of the articles included in this systematic review show that the approach experimental is the most dominant method used in related research Surface engineering of nanocrystals on quantum dot solar cells (QDSCs). Of the total articles reviewed, 20 studies used experimental methods to test the effects of surface techniques such as ligand exchange, passivation, and the formation of structures core-shell on photovoltaic performance and charge carrier dynamics. The dominance of these methods indicates that QDSCs studies rely heavily on empirical approaches to evaluate key parameters such as photovoltaic efficiency, carrier lifetime, and recombination rate, which is directly affected by the surface conditions of the nanocrystals.

Besides that, 5 articles use theoretical analysis which usually involve quantum physics approaches, recombination theory, and band structure models to explain the phenomena

occurring at nanocrystal interfaces. These studies play an important role in strengthening the conceptual understanding of the interaction mechanisms between surfaces and charge carriers, especially in the context of trap states And surface defect density.

Simulation study, which includes 4 articles, utilizing numerical modeling and photovoltaic simulation software (such as SCAPS-1D or TCAD) to predict the behavior of QDSCs systems with different surface conditions. These simulations are useful for testing hypotheses before experimental implementation and allow the analysis of parameters that are difficult to measure directly in the laboratory. Meanwhile, 3 articles which belong to review articles provide a summary of the research trends, challenges, and potentials in this field, but does not specifically link surface engineering techniques to charge dynamics in depth. This strengthens the argument that there is still a literature gap in terms of a comprehensive and systematic review of this aspect.

Finally, there are 2 case studies that discuss specific applications of QDSCs in the context of specific devices or environments, such as application on flexible substrates or integration with hybrid solar panel systems. Although limited in number, these case studies demonstrate the potential for practical applications of surface engineering research results.Overall, the dominance of experimental studies underscores the urgency of integrating these empirical findings into a more systematic conceptual framework, as attempted in this research. The combination of experimental results, theory, and simulations is crucial for formulating optimal surface engineering strategy, with direct implications for improving the efficiency and long-term stability of QDSCs.

3.1.5. Journal Database Sources

Tabel 4. Journal Database Sources

Database	Number of Articles
Scopus	22
Web of Science	12

Source: Processed Data, 2025

In the process of compiling this systematic literature review, the selection of credible scientific databases is a crucial aspect to ensure that the reviewed studies have high academic standards. Of the total articles collected and analyzed, the majority came fromScopus with the number 22 articles, followed by Web of Science (WoS) as much as 12 articles. The use of these two databases not only reflects the breadth of the search, but also reflects an effort to reach the literature that is high quality and verified through a rigorous peer-review process.

Scopus, as one of the largest and most widely used databases in academia, covers a wide range of journals from engineering, science, and energy disciplines. Many studies in Scopus examine the topic quantum dot solar cells (QDSCs)from experimental aspects to the latest technological applications, including engineering nanocrystal surface engineering like ligand exchange, passivation, And core-shell engineering.

Meanwhile, Web of Science Adds depth to this study through coverage of journals with a specific focus on material science, photonics, And nanotechnology. The studies obtained from WoS enrich the thematic analysis and help identify global trends inQDs surface innovations that directly correlate with increased photovoltaic efficiency and charge dynamics.

The concentration of literature on these two main sources also provides justification that this research is built on solid and reliable foundation of literature, while also showing that

the topic of QDSCs and surface engineering has attracted the attention of the scientific community across disciplines and countries. This distribution strengthens the systematic validity of the research and supports the quality of analysis and generalization of the findings.

3.1.6. Theories Used in Research

Tabel 5. Theories Used in Research

Theory Name	Number of Articles
Quantum Mechanics	15
Photovoltaic Theory	10
Semiconductor Physics	5
Nanotechnology	4

Source: Processed Data, 2025

Analysis of the reviewed articles showed that studies onQuantum Dot Solar Cells (QDSCs)relies heavily on a multidisciplinary theoretical framework. In general, there are four main theories that are most widely used, namelyQuantum Mechanics, Photovoltaic Theory, Semiconductor Physics, And Nanotechnology, with their respective distributions 15, 10, 5, And article.

Quantum Mechanics Dominates as the most frequently used theory (15 articles), considering that the working principle of quantum dots intrinsically involves phenomena quantum confinement, discrete energy levels, And tunneling effect. Understanding the dynamics of charge, including the processes of excitation, relaxation, and the movement of electrons and holes at the nanoscale level, cannot be explained without a quantum approach. This theory is the main foundation for explaining how nanocrystal surface engineering can affect the efficiency of solar cells through control overstates density And interface trap levels.

Meanwhile, Photovoltaic Theory is used in 10 articles as a framework for understanding conversion of light energy into electrical energy through the mechanisms of charge generation, separation, and collection. In the context of surface engineering, this theory is relevant to explain the impact of changes in surface chemistry or morphology on performance parameters such as open-circuit voltage (Voc), short-circuit current (Jsc), And power conversion efficiency (PCE).

Semiconductor Physics, used in 5 articles, supports the analysis of energy band structures (bandgap engineering), charge mobility, and recombination effects. This theory bridges the understanding from quantum aspects to macroscopic phenomena in QD-based semiconductor materials, especially in explaining the effects of passivation And ligand exchange on load transport performance.

Finally, Nanotechnology Presented in 4 articles to emphasize aspects of nanomaterial structure design and fabrication, as well as surface modification techniques that utilize nanoscale chemical and topological functions. The presence of this theory shows the importance of material engineering technology approach in manipulating surface structure to reduce defects and improve operational stability of QDSCs.

Overall, these four theories complement each other and forman integral conceptual framework in answering this research question:how nanocrystal surface engineering affects charge dynamics and photovoltaic efficiency in QDSCs. This multidisciplinary approach strengthens the theoretical validity of the research and provides a strong foundation for further exploration in the design and optimization of quantum dots-based solar cells.

3.2 Key Findings

Thematic analysis resulted in three main categories that summarize the focus of findings from all the studies reviewed:

1. Surface Engineering Techniques

There are three main approaches in the surface engineering of QDs:

- **Ligand Exchange:** The process of replacing long organic ligands with short or inorganic ligands to increase conductivity and inter-dot proximity. This technique has been shown to reduce interparticle distances, strengthen electronic bonds, and accelerate charge transfer.
- **Surface Passivation:** This strategy aims to cover up or eliminate surface trap states which are the centers of non-radiative recombination. The use of materials such as halide ions, thiols, and ammonium salts has been shown to be effective in reducing trap density and increasing optoelectronic stability.
- **Core-Shell Structures:** This technique involves coating the core QDs with a shell material that is compatible in terms of bandgap and structure. This structure is able to inhibit recombination at the surface and prolong the lifetime of charge carriers.

2. Impact on Load Dynamics

Almost all studies show that surface modification of QDs significantly:

- Increases the lifetime of charge carriers, allowing a longer time for the charge to reach the electrodes.
- Reducing electron-hole recombination, both radiative and non-radiative, by suppressing the presence of trap states on the surface.
- Increase mobility and charge diffusion, especially in layer configurations that have undergone ligand engineering processes.

3. Relationship between Surface Structure and Photovoltaic Efficiency

Surface engineering has a direct contribution to three key parameters of photovoltaic performance:

- Voc (open-circuit voltage) increases due to the reduction in level mid-gap traps that usually cause recombination loss.
- Jsc (short-circuit current) increases as the efficiency of absorption and charge transport becomes more optimal.
- PCE (power conversion efficiency) shows significant improvement, especially in studies combining more than one surface engineering technique.

Several studies have noted a jump in efficiency from around 4–5% to 10–13% after applying double passivation techniques and using short inorganic-based ligands.

4. DISCUSSIONS

4.1 Synthesis of Results

The performance of quantum dot solar cells (QDSCs) is significantly influenced by various surface engineering techniques that optimize charge dynamics, enhance charge carrier mobility, and reduce recombination centers, thereby directly correlating with improved photovoltaic efficiency. One of the pivotal strategies in surface engineering is ligand exchange, wherein long organic ligands are replaced with shorter inorganic counterparts. This substitution has been shown to lower interfacial resistance and improve the electrical connectivity between quantum dots and the charge transport layer. For instance, Ren et al. demonstrated that the use of thiosulfate-capped quantum dots led to a notable enhancement in photovoltaic performance, achieving a power conversion efficiency (PCE) of 6.11%, indicating the effectiveness of ligand manipulation in optimizing QDSCs (Ren et al., 2017). Similarly, Wheeler

et al. highlighted that ligand exchange with halides produced defect-free quantum dot arrays, which are critical in producing high-efficiency solar cells (Wheeler et al., 2018). These findings suggest that effective surface engineering through ligand modification plays a crucial role in enhancing charge transport and reducing recombination.

Surface passivation is another significant technique that enhances the quality of the quantum dot interface. Passivation methods, particularly using halide ions, effectively close surface defects, thereby increasing carrier lifetimes and mobility. Huang et al. illustrated how hybrid passivation utilizing mercaptopropionic acid (MPA) improved the efficiency and stability of QDSCs significantly, confirming that the reduction of trap states is critical for optimizing performance (Huang et al., 2014). Furthermore, studies by Sloboda et al. provided evidence that interface engineering can directly influence photovoltage generation and decay dynamics, emphasizing the importance of regulating surface traits to achieve superior charge transfer properties (Sloboda et al., 2024).

The formation of core-shell structures is yet another approach that contributes to the enhancement of QDSC efficiency. By creating such structures, the band alignment can be effectively controlled, providing superior electronic properties that facilitate charge transport. Pan et al. reported on the successful application of a core-shell architecture using modified deposition techniques, achieving a remarkable PCE of 5.32% for their CdS/CdSe-sensitized solar cells (Pan et al., 2012). This trend indicates that tailor-made nanostructures can profoundly affect charge dynamics and overall solar cell efficiency. In conclusion, the optimization of surface structures through techniques like ligand exchange, surface passivation, and core-shell engineering is essential not only for improving the interface quality between quantum dots and transport layers but also for enhancing charge carrier mobility and diminishing trap states. These improvements collectively bolster the functional architecture of QDSCs, underscoring the significance of surface engineering as a foundational element in the development of efficient photovoltaic technologies.

4.2 Theoretical and Practical Implications

From a theoretical perspective, these findings strengthen existing models related to interface state density and recombination dynamics in nanocrystal systems. In the context of QDSCs, the nanocrystal surface is the primary location for the formation of trap states, which can act as non-radiative recombination centers. By reducing the density of these traps through surface engineering, adjustments are made to the Fermi level position and improved energy band alignment, which directly impacts the increase in open-circuit voltage (V_{oc}).

From a practical perspective, the results of this study provide a solid foundation for the development of more efficient and stable QDSCs designs. The selection of appropriate surface engineering techniques, tailored to the type of quantum dots and the final application, enables the creation of high-performance photovoltaic systems with process complexity that remains manageable. In addition, the combination of surface engineering techniques also opens up the potential for the integration of QDSCs in flexible electronics and building-integrated photovoltaics (BIPV) devices, which require high efficiency as well as long-term stability.

4.3 Comparison with Previous Studies

The study of charge carrier dynamics in quantum dot solar cells (QDSCs) is crucial for advancing their efficiency and optimization. This particular research contributes significantly by establishing the causal relationship between surface engineering techniques and charge carrier dynamics, an area that prior literature has largely neglected. Most existing studies have predominantly been concerned with material synthesis and efficiency metrics without linking the nuanced impacts of surface structure on photovoltaic parameters such as charge mobility, carrier lifetime, and trap-assisted recombination. One of the fundamental insights provided by this research is how modifications in surface characteristics can influence charge trapping

dynamics. For instance, Pollock and Schlenker elucidate that charge trapping greatly affects the electron and hole lifetimes in perovskite solar cells, with higher trap state densities correlated negatively with device performance (Pollock & Schlenker, 2021). Additionally, they describe the correlation between conduction band electron lifetime and the charge trapping parameters, further emphasizing the necessity of considering these dynamics for optimizing device efficiency (Pollock & Schlenker, 2019). The study by Santra and Kamat discusses the tuning of the photovoltaic response through surface structuring in tandem-layered QDSCs, thereby demonstrating how charge separation aligns with surface features, although it does not explicitly focus on charge dynamics (Santra & Kamat, 2013).

Moreover, prompted by the findings of Fu et al., it becomes apparent that the interactions among charge carriers and quantum dots are significantly influenced by electrode structure as well, which directly relates to their photovoltaic performance (Fu et al., 2021). Their results indicate that the charge injection and transition processes within the structure have pivotal roles in overall efficiency, reinforcing the argument for a mechanistic understanding of charge dynamics. Furthermore, the work of Tian et al. contributes to understanding the charge recombination pathways in QDSCs, revealing that interface resistance and the morphological arrangement of quantum dot layers considerably modify charge separation efficiencies (Tian et al., 2013). These insights help fill the observed gap in the literature—where the interplay between surface characteristics and charge dynamics remains understudied—by elaborating on the significance of optimal surface engineering. The integration of insights from various studies helps underscore the overall narrative that improving photovoltaic performance in QDSCs necessitates a comprehensive understanding of the surface engineering techniques and their direct correlation with charge carrier dynamics. By systematically mapping these relationships, the present study lays a robust foundation for adopting mechanism-driven design approaches in future QDSC developments.

4.4 Study Limitations

Although the selection of articles followed a systematic procedure, this study still has several limitations. First, the existence of publication bias, where only articles with positive or significant results tend to be published, may lead to overestimation of the effectiveness of certain techniques. Second, limitations in the use of keywords may lead to missing relevant articles that use different technical terms. Third, not all articles use uniform measurement parameters; for example, some only report efficiency without including lifetime or recombination rate data, making it difficult for a more in-depth comparative analysis.

4.5 Recommendations for Further Research

Based on the findings and limitations, there are several important directions for further research:

1. **Interdisciplinary Approach**
Future research should integrate materials science, photonics, and quantum computing to model and simulate surface effects more precisely. The use of *ab initio* simulations or non-adiabatic molecular dynamics can provide atomistic insights into charge transfer at nanocrystal interfaces.
2. **Influence of Operational Environment**
Future studies should also consider the environmental effects, such as humidity, temperature, and UV exposure, on the stability of engineered surfaces. This is important considering that many QDSCs experience efficiency degradation when operated under real-world conditions, especially those based on perovskite QDs.
3. **Long-Term Evaluation and Replication**
Long-term stability and reproducibility studies of surface engineering results are needed, especially in the context of scalability and mass production. Some techniques

may show high performance in the laboratory, but are not compatible with industrial-scale manufacturing processes.

5. CONCLUSION

5.1 Summary of Key Findings

This systematic review confirms that nanocrystal surface engineering plays a crucial role in improving the performance of quantum dot solar cells (QDSCs). Through an analysis of relevant literature from 2012 to 2024, it was found that strategies such as ligand exchange, surface passivation, and the formation of core-shell structures can consistently improve the charge carrier dynamics, extend the carrier lifetime, and reduce the non-radiative recombination rate. The implications of these improvements are reflected in the increase of key photovoltaic parameters, such as open-circuit voltage (Voc), short-circuit current density (Jsc), and power conversion efficiency (PCE). Thus, surface engineering not only improves the interactions at the material interface but also becomes an important foundation for the design of next-generation solar cells.

5.2 Contribution to the Literature

This study makes a significant contribution to the development of science in the field of nanocrystal-based photovoltaics, especially through providing a conceptual framework that explains the systematic relationship between surface engineering techniques and charge transport mechanisms and dynamics. In addition, this study produces a literature map that groups the main surface engineering strategies and their impacts on the performance of QDSCs. Thus, this study can be an important reference for material scientists, renewable energy researchers, and photovoltaic technology developers in understanding and optimizing QDSCs designs in a more focused and empirically evidence-based manner.

5.3 Study Limitations

Although the approach used is systematic and based on the PRISMA framework, there are several limitations that need to be noted. First, the literature selection was limited to English-language articles, potentially excluding important research in other languages. Second, only four major databases were used (Scopus, Web of Science, ScienceDirect, and IEEE Xplore), so there is a possibility that other sources are relevant that have not been covered. Third, variations in methodology, measurement parameters, and terminology across studies may affect the level of consistency in the comparative analysis.

5.4 Suggestions for Future Research

To strengthen the scientific foundation and application of surface engineering strategies in QDSCs, further research is suggested to explore:

- A multi-functional surface design that not only increases charge efficiency, but also provides resistance to degradation due to environmental factors such as humidity, extreme temperatures, or UV exposure.
- Integration of artificial intelligence (AI) and machine learning in developing predictive models for nanocrystal surface optimization. These models can be used to virtually screen ligand combinations and passivation methods before physical experiments, thus accelerating the process of efficient new material discovery.
- A multidisciplinary collaboration between the fields of materials science, physical chemistry, and computational engineering to create a deeper understanding of structure-surface-function correlations.

By combining experimental, theoretical, and computational approaches, the future of efficient and sustainable QDSCs can be realized more rapidly and scalably.

6. REFERENCE

- Arxiv. (2016). Halide-terminated quantum dots suppress electron–phonon coupling. Retrieved from <https://arxiv.org/abs/1611.09930>
- Cappelluti, F., Niemi, T., Guinã, M., Kim, D., Wu, J., Liu, H., ... & Aho, T. (2017). Enabling high-efficiency inas/gaas quantum dot solar cells by epitaxial lift-off and light management.. <https://doi.org/10.1109/pvsc.2017.8366631>
- Fu, W., Pan, J., Niu, J., Fu, Y., Xiao, G., Wang, J., ... & Li, C. (2021). A transparent photovoltaic device of nio/mgo quantum dots/tio2 arrays pn junction with carrier injection of mgo qds. *Journal of Materials Science Materials in Electronics*, 33(2), 652-662. <https://doi.org/10.1007/s10854-021-07333-z>
- Hao, M., Bai, Y., Zeiske, S., Ren, L., Liu, J., Yuan, Y., ... & Wang, L. (2020). Ligand-assisted cation-exchange engineering for high-efficiency colloidal cs1–xfaxpbi3 quantum dot solar cells with reduced phase segregation. *Nature Energy*, 5(1), 79-88. <https://doi.org/10.1038/s41560-019-0535-7>
- Huang, J., Xu, B., Yuan, C., Chen, H., Sun, J., Sun, L., ... & Ågren, H. (2014). Improved performance of colloidal cdse quantum dot-sensitized solar cells by hybrid passivation. *Acs Applied Materials & Interfaces*, 6(21), 18808-18815. <https://doi.org/10.1021/am504536a>
- Jia, D., Chen, J., Zheng, S., Phuyal, D., Yu, M., Tian, L., ... & Zhang, X. (2019). Highly stabilized quantum dot ink for efficient infrared light absorbing solar cells. *Advanced Energy Materials*, 9(44). <https://doi.org/10.1002/aenm.201902809>
- Jin-nouchi, Y., Naya, S., & Tada, H. (2010). Quantum-dot-sensitized solar cell using a photoanode prepared by in situ photodeposition of cds on nanocrystalline tio2 films. *The Journal of Physical Chemistry C*, 114(39), 16837-16842. <https://doi.org/10.1021/jp1062226>
- Kong, E., Joo, S., Park, H., Song, S., Chang, Y., Kim, H., ... & Jang, H. (2014). Bandgap tuning with thermal residual stresses induced in a quantum dot. *Small*, 10(18), 3678-3684. <https://doi.org/10.1002/sml.201400392>
- Kramer, I. and Sargent, E. (2011). Colloidal quantum dot photovoltaics: a path forward. *Acs Nano*, 5(11), 8506-8514. <https://doi.org/10.1021/nn203438u>
- Li, Q., Jin, X., Yang, Y., Wang, H., Xu, H., Cheng, Y., ... & Luo, S. (2015). Nd2(s, se, te)3 colloidal quantum dots: synthesis, energy level alignment, charge transfer dynamics, and their applications to solar cells. *Advanced Functional Materials*, 26(2), 254-266. <https://doi.org/10.1002/adfm.201503433>
- Nozawa, T., Takagi, H., Watanabe, K., & Arakawa, Y. (2015). Direct observation of two-step photon absorption in an inas/gaas single quantum dot for the operation of intermediate-band solar cells. *Nano Letters*, 15(7), 4483-4487. <https://doi.org/10.1021/acs.nanolett.5b00947>
- Ozu, S., Zhang, Y., Yasuda, H., Kitabatake, Y., Toyoda, T., Hirata, M., ... & Shen, Q. (2019). Improving photovoltaic performance of zno nanowires based colloidal quantum dot solar cells via sno2 passivation strategy. *Frontiers in Energy Research*, 7. <https://doi.org/10.3389/fenrg.2019.00011>
- Pan, Z., Zhang, H., Cheng, K., Hou, Y., Hua, J., & Zhong, X. (2012). Highly efficient inverted type-i cds/cdse core/shell structure qd-sensitized solar cells. *Acs Nano*, 6(5), 3982-3991. <https://doi.org/10.1021/nn300278z>
- Pitchaimuthu, S., Chandramohan, S., Kumar, R., Sathyamoorthy, R., Hong, C., & Kang, Y. (2010). Fabrication and charge-transfer characteristics of cds qds sensitized vertically grown flower-like zno solar cells with cdse cosensitizers. *Physica Status Solidi (A)*, 208(2), 474-479. <https://doi.org/10.1002/pssa.201026276>
- Pollock, T. and Schlenker, C. (2019). Electromodulation and transient absorption spectroscopy suggest conduction band electron lifetime, electron trapping parameters, and

- ch₃nh₃pbi₃ solar cell fill factor are correlated. *The Journal of Physical Chemistry C*, 123(30), 18160-18170. <https://doi.org/10.1021/acs.jpcc.9b02748>
- Pollock, T. and Schlenker, C. (2021). Charge trapping dynamics revealed in ch₃nh₃pbi₃ by ultrafast multipulse spectroscopy. *The Journal of Physical Chemistry C*, 125(34), 18834-18840. <https://doi.org/10.1021/acs.jpcc.1c05513>
- PV Magazine. (2022, September 14). Perovskite quantum dot solar cell with 16.25% efficiency. Retrieved from <https://www.pv-magazine.com/2022/09/14/perovskite-quantum-dot-solar-cell-with-16-25-efficiency/>
- Ren, Z., Yu, J., Pan, Z., Wang, J., & Zhong, X. (2017). Inorganic ligand thiosulfate-capped quantum dots for efficient quantum dot sensitized solar cells. *Acs Applied Materials & Interfaces*, 9(22), 18936-18944. <https://doi.org/10.1021/acsami.7b03715>
- Rühle, S., Shalom, M., & Zaban, A. (2010). Quantum-dot-sensitized solar cells. *Chemphyschem*, 11(11), 2290-2304. <https://doi.org/10.1002/cphc.201000069>
- Santra, P. and Kamat, P. (2012). Mn-doped quantum dot sensitized solar cells: a strategy to boost efficiency over 5%. *Journal of the American Chemical Society*, 134(5), 2508-2511. <https://doi.org/10.1021/ja211224s>
- Santra, P. and Kamat, P. (2013). Tandem-layered quantum dot solar cells: tuning the photovoltaic response with luminescent ternary cadmium chalcogenides. *Journal of the American Chemical Society*, 135(2), 877-885. <https://doi.org/10.1021/ja310737m>
- Shu, G. (2024). Progress of advanced quantum dots and their applications in quantum dot sensitized solar cells. *Highlights in Science Engineering and Technology*, 111, 246-252. <https://doi.org/10.54097/4shn3e59>
- Sloboda, T., Kammlander, B., Berggren, E., Riva, S., Giangrisostomi, E., Ovsyannikov, R., ... & Cappel, U. (2024). Interface-resolved photovoltage generation dynamics and band structure evolution in a pbs quantum dot solar cell. *Nanoscale*, 16(45), 21002-21010. <https://doi.org/10.1039/d4nr03428g>
- Sun, M., Zhu, D., Ji, W., Jing, P., Li, L., Xiang, W., ... & Zhao, J. (2013). Exploring the effect of band alignment and surface states on photoinduced electron transfer from cuins₂/cds core/shell quantum dots to tio₂ electrodes. *Acs Applied Materials & Interfaces*, 5(23), 12681-12688. <https://doi.org/10.1021/am4040224>
- Tang, J. and Sargent, E. (2010). Infrared colloidal quantum dots for photovoltaics: fundamentals and recent progress. *Advanced Materials*, 23(1), 12-29. <https://doi.org/10.1002/adma.201001491>
- Technology Networks. (2024, January 9). Researchers Develop World's Most Efficient Quantum Dot Solar Cells. Retrieved from <https://www.technologynetworks.com/cell-science/news/researchers-develop-worlds-most-efficient-quantum-dot-solar-cells-384131>
- Tian, J., Zhang, Q., Uchaker, E., Liang, Z., Gao, R., Qu, X., ... & Cao, G. (2013). Constructing znO nanorod array photoelectrodes for highly efficient quantum dot sensitized solar cells. *Journal of Materials Chemistry A*, 1(23), 6770. <https://doi.org/10.1039/c3ta11056g>
- Tian, J. and Cao, G. (2013). Semiconductor quantum dot-sensitized solar cells. *Nano Reviews*, 4(1), 22578. <https://doi.org/10.3402/nano.v4i0.22578>
- Unluler, M. and Koç, F. (2024). Comparative analysis of excitonic and biexcitonic effects on the power conversion efficiency of a cdse/cdte/znte quantum dot solar cell. *Advanced Theory and Simulations*, 8(3). <https://doi.org/10.1002/adts.202400956>
- Unluler, M. and Koç, F. (2024). Comparative analysis of excitonic and biexcitonic effects on the power conversion efficiency of a cdse/cdte/znte quantum dot solar cell. *Advanced Theory and Simulations*, 8(3). <https://doi.org/10.1002/adts.202400956>

- Wei, H., Li, D., Zheng, X., & Meng, Q. (2018). Recent progress of colloidal quantum dot based solar cells. *Chinese Physics B*, 27(1), 018808. <https://doi.org/10.1088/1674-1056/27/1/018808>
- Wheeler, L., Sanehira, E., Marshall, A., Schulz, P., Suri, M., Anderson, N., ... & Luther, J. (2018). Targeted ligand-exchange chemistry on cesium lead halide perovskite quantum dots for high-efficiency photovoltaics. *Journal of the American Chemical Society*, 140(33), 10504-10513. <https://doi.org/10.1021/jacs.8b04984>
- Xue, J., Lee, J., Dai, Z., Wang, R., Nuryyeva, S., Liao, M., ... & Yang, Y. (2018). Surface ligand management for stable fapbi3 perovskite quantum dot solar cells. *Joule*, 2(9), 1866-1878. <https://doi.org/10.1016/j.joule.2018.07.018>
- Yang, Z., Chen, C., Roy, P., & Chang, H. (2011). Quantum dot-sensitized solar cells incorporating nanomaterials. *Chemical Communications*, 47(34), 9561. <https://doi.org/10.1039/c1cc11317h>
- Yuan, J., Ling, X., Yang, D., Li, F., Zhou, S., Shi, J., ... & Ma, W. (2018). Band-aligned polymeric hole transport materials for extremely low energy loss α -cspbi3 perovskite nanocrystal solar cells. *Joule*, 2(11), 2450-2463. <https://doi.org/10.1016/j.joule.2018.08.011>
- Zhang, X., Cappel, U., Jia, D., Zhou, Q., Du, J., Sloboda, T., ... & Johansson, E. (2019). Probing and controlling surface passivation of pbs quantum dot solid for improved performance of infrared absorbing solar cells. *Chemistry of Materials*, 31(11), 4081-4091. <https://doi.org/10.1021/acs.chemmater.9b00742>