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Research Article

The Frontier of Solar Energy: Quantum Dots and Density Functional Theory Insights

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ABSTRACT

Solar cells, a crucial renewable energy source in the fight against climate change, have gained prominence in the scientific community. Sunlight, an almost inexhaustible source of clean and renewable energy, positions solar cells as a fundamental alternative for future energy needs. However, improving their energy efficiency remains a major challenge. Quantum dots, nanocrystals with unique properties, have emerged as a promising solution due to their ability to harvest a wider range of light wavelengths. Despite challenges in producing these cells, computational simulation tools based on Density Functional Theory (DFT) offer a robust theoretical framework. These tools provide a low-cost way to elucidate the internal processes of energy conversion, thereby accelerating development. The existing literature on this topic is scarce and dispersed, underscoring the need for research to consolidate key contributions. This article employs scientometric techniques to identify seminal works and analyze the dynamics in the scientific production of quantum dot-based solar cells. The results reveal a surge in research activity, particularly in the last three years, highlighting the growing interest in this promising technology. Moreover, results show a 38.95% growth between 2012 and 2019, with an upward trend in scientific production. China and the United States of America lead academic production in this field. Three well-defined trends in the development of quantum dot-based solar cells are identified: Halide perovskites, dye-sensitized, and nanocrystals. These findings can assist researchers in gaining a better understanding of the current research landscape and trends in this field.

Keywords: Solar cell, Quantum dot, Density functional theory, Perovskite, Dye sensitized.

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INTRODUCTION

Solar energy has emerged as a promising alternative to traditional energy sources. Various methods exist for capturing this energy, but Quantum Dot-based Solar Cells (QDSCs) stand out for their high efficiency potential and growth expectations in the global market.[1] The integration of Quantum Dots (QDs) into photovoltaic devices has opened new horizons for increasing light absorption efficiency. Simulation tools based on Density Functional Theory have become an essential tool for comprehending and predicting the electronic properties of QDs at the atomic level.

QDs are semiconductor particles at the nanometer scale that can convert light energy into electrical energy with greater efficiency than other alternatives.[2] For example, QDs display a quantum confinement effect, which allows for the control of their optical and electronic properties by adjusting their size.[3] Additionally, they can produce multiple excitons from a single high-energy photon,[4] potentially resulting in solar cell efficiencies that exceed the Shockley-Queisser limit.[5] In addition, QDs have a significantly larger absorption cross-section than bulk material, allowing them to absorb more light. Moreover, QDs can be processed and synthesized in solution, enabling low-cost manufacturing techniques such as spin-coating.[6] Therefore, it is essential to conduct research on alternative energies, such as QDSCs, to reduce dependence on traditional energy sources.

Recently, theories have been developed to understand and improve the designs of QDSCs, such as DFT. The DFT enables the

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prediction of electronic structure, formation energies, magnetic, and optical properties of materials. This theory facilitates the calculation of energy band structures of semiconductor materials, providing insights into electronic and optical bandgaps. This process is essential for the optimal design of semiconductors with higher efficiencies for solar cells. Moreover, DFT predicts absorption and emission energy transitions, offering details on crystalline lattice defects.[7] Through DFT, it is possible to understand how these defects affect the electronic charge density, impacting the recombination of charge carriers and photovoltaic efficiency.

While the importance of solar cells and enhancing their efficiency is recognized, academic literature has exponentially grown in recent years and lacks studies that consolidate key contributions and the dynamics of scientific production. According to our search, very few review studies were found, none utilizing quantitative strategies. For instance, Liang *et al.*,[8] conducted a review on graphene advancements for solar cell applications. Al-Douri *et al.*,[9] focused on identifying key contributions in QDs synthesis and properties in solar cells. Lastly, Manzhos *et al.*,[10] conducted a more general study to identify the latest technologies in designing materials for next-generation solar cells. None of these studies compiled quantitative data, nor focused on DFT. Therefore, this is the first review with a scientometric focus on QDSCs.

This study combines scientometric analysis and computational approach to comprehensively analyze the evolution of research on Quantum Dot Solar Cell (QDSC). Using data from Scopus and Web of Science databases, we performed a detailed bibliometric analysis, including authorship networks, country-wise collaboration patterns, and keyword co-occurrence to identify key research trends and influential contributors in the field. The application of scientiometric approaches to uncover research dynamics has also been successfully demonstrated in other areas, such as pulmonary diseases, highlighting the versatility and value of these methodologies in diverse scientific fields.[11,12] In this study, the ToS[13,14] algorithm was used to identify foundational articles, key contributions that have shaped the development of QDSCs, and emerging research trends. Together, these analyses provide a comprehensive overview of the QDSC research landscape and inform future research directions. The following sections detail the methodology, results, and conclusions.

METHODOLOGY

The parameters for the scientometric search QDSCs using DFT are detailed in Table 1. Data were retrieved from WoS and Scopus on January 1, 2024. Keywords were grouped into the three themes of this study. Results indicated that most of the scientific production was found in Scopus. However, following current scientometric trends,[15,16] results from both databases were utilized to achieve broader coverage (10.79% of the total articles were not found in Scopus). Articles, books, chapters, and conference papers were included as these document types hold significance in certain knowledge areas.[17]

Compared to other review methods, scientometric analysis relies on quantitative analysis of the scientific literature. These results provide an overview of the existing literature on a particular topic, offering the advantage of rigor and reduced bias, and thus serve as a complement to other qualitative review methods.

Figure 1 shows an adaptation of the PRISMA flowchart. Preprocessing was one of the most important steps in the methodology. It was a complex process due to formatting differences between WoS and Scopus; for example, references in WoS include DOIs, while those in Scopus have comprehensive information but vary in citation format. Web scraping and text mining were required to standardize the references. Since WoS references include DOIs, these were used to capture additional data information not presented in WoS downloads through the Crossref platform. Text mining was also used to standardize Scopus references to extract authors, journals, and years. This process enriches the analysis and allows for more precise explanations of the resulting figures. The result was an Excel file with 22 sheets of organized information ready for analysis and graph generation from both databases. The detailed scientometric analysis and the application of the ToS algorithm are explained below.

Scientometric Analysis

The scientometric analysis was divided into the following sections: scientific production, countries, journals, and authors. This approach begins with a general overview and ends with a more detailed examination through the author analysis. The country, journal, and author analyses are divided into two parts. The first provides a broad perspective through tabular analysis, while the second highlights the relationships between different entities. For the analysis of scientific collaboration, the approach proposed by Hurtado-Marín *et al.*,[18] which includes authors from references for network construction, was followed. This novel method of analyzing scientific collaboration networks allows a better understanding of networking strategies within a scientific community.[19]

Tree of Science

The ToS algorithm is based on the process of raw and elaborated sap flow in a plant.[20] After citation network construction, the algorithm identifies articles at the root and trunk based on a metric called SAP, which ranges from roots to leaves and then returns to enhance results. This algorithm has been utilized across various fields including marketing,[21,22] entrepreneurship,[23] environment,[24] tourism,[25] and psychology.[26,27] The tool was launched in 2015 and is currently available at the following link https://tos.coreofscience.org/.[13] The ToS algorithm is designed to complement other tools like VOSviewer and Bibliometrix. We

chose ToS for its user-friendly approach to identifying relevant articles within a research area based on keyword selection (Table 1).

RESULTS AND DISCUSSION

Scientometric Analysis

Scientific production

Analyzing annual scholarly production is crucial for understanding how research on the QDSCs has evolved over time. As shown in Figure 2, this analysis allows us to track publication trends in databases like Scopus and WoS over the past 22 years. There is a notable difference in production between the two databases, with Scopus dominating throughout the period (green bar). However, the unified production (red line) shows that since 2014, WoS has contributed unique articles not found in Scopus. This underlines the importance of considering both databases for reviews and scientometric analyses. Moreover, there is a significant increment in the article production in the Scopus database since 2015. Citations received show three significant peaks in 2012, 2014, and 2017, along with the lag effect typical of citation behavior after 2019. The annual growth during this period was 14.68%, indicating a renewed interest among researchers in the study and improvement of solar panel efficiency. Three periods were divided based on the annual growth percentage, which will be explained below.

Starting period (2000-2011)

During this period, there was a growth of 16.95%, with zero production values in the years 2000, 2001, 2002, 2004, and 2005. However, from 2006 to 2011, scientific articles related to QDSCs began to be published.

Growth period (2012-2019)

This period was characterized by a rapid growth of 38.95%. Both WoS and Scopus contributed significantly to the subject. The highest peak of citations occurred in 2012, due to the application of DFT and modelling of optoelectronics devices to improve the performance of solar cells.[28] In 2014, the peak of citations received was due to several studies related to contributions using QDs and graphene.[29]

Stabilization period (2020-2022)

This period shows a renewed interest in solar cells with a growth of 26.03%. The decrease in scientific production in 2020 may be due to the global pandemic, which limited laboratory experiments. However, by 2022, production is almost equal to the highest production in 2018, indicating significant or better growth in the coming years.

Country Analysis

Country analysis based on researcher affiliation allows the identification of government efforts in scientific topics. For example, Table 2 shows the top ten countries for scientific production of QDSCs, along with the impact measured in citations received and quality measured in Scimago quartiles. The scientific production is led by China with 26.49% (71), followed by the USA with 17.16% (46). It is noteworthy that although China's production is 1.5 times that of the US, the citation percentages for both countries are not significantly different (30.21% vs. 26.23%). This suggests that while China is producing larger volume of research, the USA continues to make substantial and influential contributions to the field of QDSC research. It is also important to note that although Saudi Arabia is ranked fifth in Table 2, it is ranked third in terms of citations received.

Recent research in China has shown that QDs can be optimized in terms of structure and energy stability, making them a viable option for improving solar cell performance.[30] On the other hand, the USA has been working on high-efficiency phosphors for the construction of white light-emitting diode devices for photovoltaic applications, which have shown good photoelectric properties.[31] In addition, researchers from India are investigating new forms of silicon carbide useful for solar cells.[32]

Scientific collaboration between countries based on authors' affiliations allows the identification of groups of countries working together (see Figure 3). The collaborative network shows three well-defined groups or communities (see Figure 3a). The first community, led by Saudi Arabia, India, and Malaysia, is the largest (see Figure 3b) and has conducted collaborative work to identify new high performance materials for QDSCs.[33] The second group is led by China and the USA, with some

Table 1: Search parameters and results for WoS and Scopus databases.

Parameters	WoS	Scopus
Range	2000 - 2023	
Date	January 1st 2024	
Document types	Articles, books, chapters, and conferences	
Words	Title-Abstract-Keywords: ("solar cell" OR ibsc OR "intermediate band solar cell") AND Title-Abstract-Keywords: ("quantum dot" OR "qd") AND Title-Abstract-Keywords: (dft OR ab-initio OR first-principles OR "first principles" OR "density functional theory")	
Results	67	248
Total (WoS+Scopus)	278	

research focused on addressing the issue of lead toxicity in solar cells by proposing lead-free oxide perovskites for photovoltaic applications.[34] The third group, led by the Netherlands and Spain, has conducted work related to addressing the cooling process of hot carriers, which results in a loss of efficiency.[35] This collaborative study demonstrated a new way to achieve efficient transfer at room temperature. An interesting aspect highlighted in the nodes and links figure over time (see Figure 3c) is the overlap of link proportions after 2016. This reflects the continuity of collaboration between the same group of countries, strengthening their relationships.

Journal Analysis

According to Table 3, journals publishing on QDSCs have the highest quality; of the top 10 journals publishing on this topic, 9 and 8 are in the highest quartile (Q1) according to the Scimago

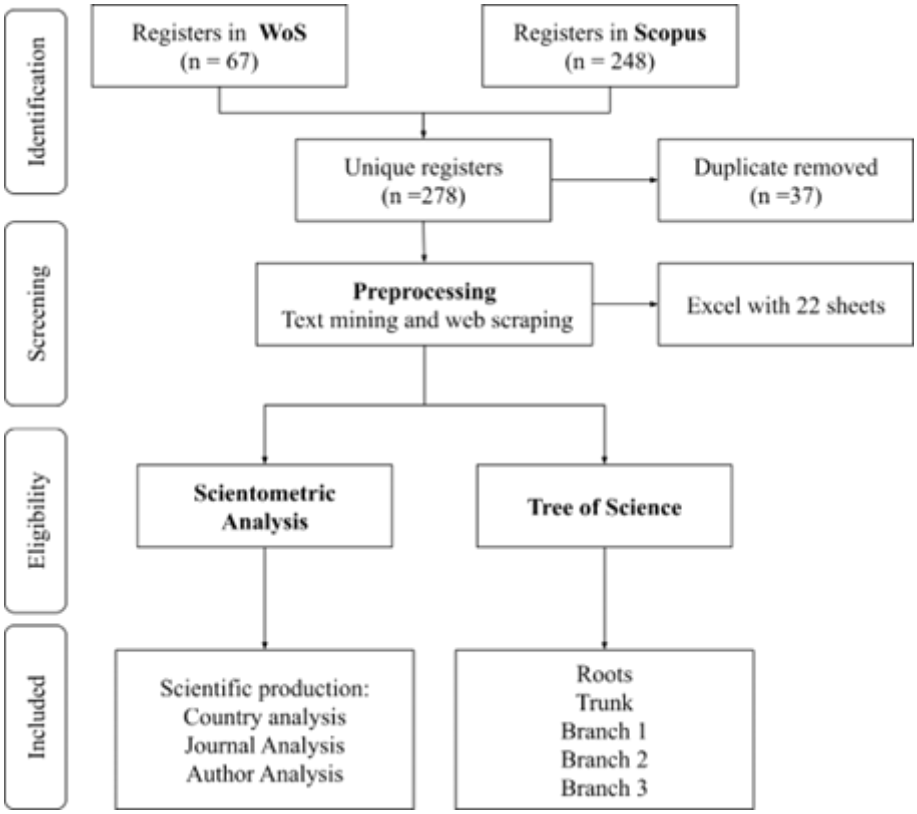

Figure 1: PRISMA flowchart for preprocessing data.

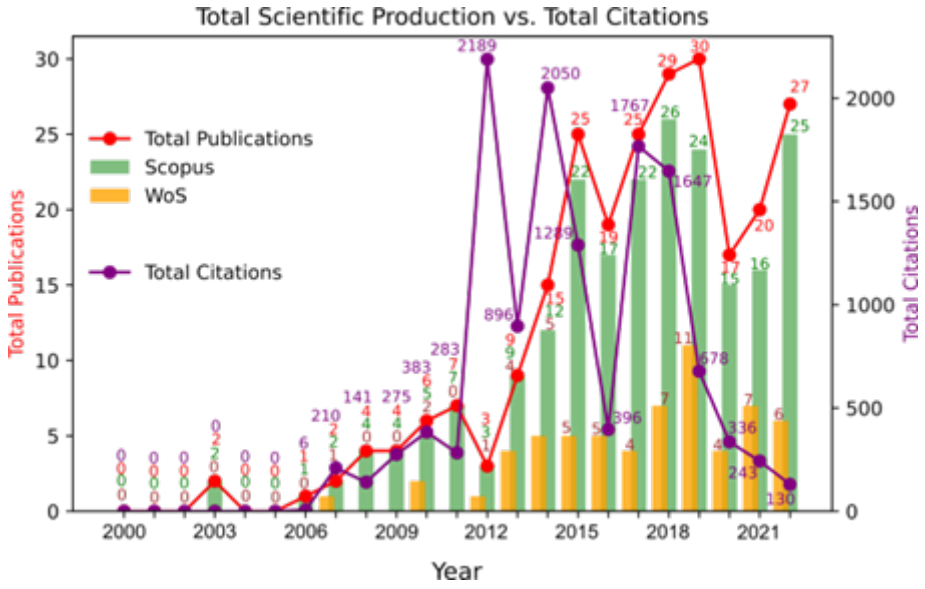

Figure 2: Correlation between annual scientific publications and total citations in quantum dot solar cell research.

Table 2: Countries by scientific production and citation.

Country	Production		Citation		Q1	Q2	Q3	Q4
China	71	26.49%	3168	30.21%	42	10	4	0
USA	46	17.16%	2750	26.23%	30	1	2	1
India	42	15.67%	515	4.91%	18	4	2	0
Spain	10	3.73%	112	1.07%	7	0	1	0
Saudi Arabia	9	3.36%	1223	11.66%	4	2	0	0
Japan	8	2.99%	126	1.2%	4	0	0	0
Iran	7	2.61%	58	0.55%	2	3	0	0
France	6	2.24%	120	1.14%	6	0	0	0
Malaysia	6	2.24%	177	1.69%	2	0	0	0
Australia	5	1.87%	96	0.92%	3	0	0	0

ranking (https://www.scimagojr.com/) and the Journal Citation Report (JCR) (https://www.webofscience.com/wos/woscc/basic-search), respectively. The Journal of Physical Chemistry C has the highest number of publications in Scopus with 22. Recently, this journal published research showing that QDs can be used for experimental design and exhibit a variety of electronic energy gaps depending on their morphology.[36] The journal with the highest H-index is the Journal Of The American Chemical Society (674), which recently published research where a MgO-QDs/TiO_2 heterojunction was designed for QDSCs, showing high light absorption efficiency, which could lead to the design of new materials for photovoltaic applications.[37]

Figure 4 shows the citation analysis between journals. Three prominent groups were identified (see Figure 4a). This analysis allows the identification of thematic groups of journals (see Figure 4b). The first group is related to materials research,[35,38] the second group emphasizes physical properties in solar cell design,[39,40] and the third group is associated with computational studies around solar cells.[9,30] The graph of nodes and links over time (see Figure 4c) shows a consolidation of topics within journals, which is reflected in the overlap of link and node proportions.

Author Collaboration Network

This section presents the top ten researchers in the field of solar cells, along with their H-index and affiliation (Table 4). Professor Long Run has the highest H-index among researchers in the field of nanoscale semiconductor development, specifically perovskites to enhance photovoltaic technologies.[41,42] Sarkar P has conducted research on simulating QDs for organic solar cells to improve its efficiency.[43,44] Researchers from around the world, particularly those affiliated with countries like China, are actively involved in this field, emphasizing the global need for advancements in alternative energy systems.

Figure 5 is created from the personal networks of researchers listed in Table 4. The network demonstrates a cohesive and consolidated community, as evidenced by the formation of a large component (blue) derived from authors' personal networks (Figure 5a). It is also noteworthy that the graph depicting (Figure 5c) nodes and links over time shows that the proportion of links surpasses the proportion of nodes (researchers) after the year 2016, indicating a strengthening of scientific collaboration. For example, although Professor Infante has conducted significant research on QD,[45,46] he has not collaborated directly with the other researchers listed in Table 4. However, his co-authors have connections with other researchers who have collaborated with some of the most productive investigators worldwide. This is reflected in the collaboration network, where authors may appear isolated from each other but remain part of the same scientific community (Figure 5b). This suggests that while there are key contributors, the overall community is interconnected, which may facilitate knowledge sharing and innovation in QDSC research.

Tree of Science

Root

The development of first-principles simulations of quantum dot-based solar cells is rooted in pioneering works. Shockley & Queisser[5] conducted one of the earliest endeavors in solar cell development, proposing a theory that established the maximum efficiency limit achievable by a p-n junction solar cell. This work paved the way for exploring alternative approaches to surpass the Shockley-Queisser limit (SQ limit). For instance, one strategy to enhance these efficiencies was through simulations. In this way, Kohn & Sham[47] established the foundation for computational calculations by introducing a method to solve the Schrödinger-like equations for many electrons using the electron charge density concept proposed by Hohenberg & Kohn.[48] The method includes Exchange and Correlation (XC) effects through an effective potential that depends on density. The authors propose a simple, efficient method for describing the electronic properties of atomic and molecular systems, which has the potential to study solid-state systems. They also emphasize the need to improve correlation treatment. Lee *et al.*,[49] proposed an

enhancement by devising a formula for Colle-Salvetti correlation energy based on electron density. The authors used the Local Density Approximation (LDA) to estimate exchange energy and electron kinetic energy functionals. They then compared the numerical results of their proposed formula with experimental data and calculations from other methods, demonstrating the validity and efficiency of their approach.

Becke[50] proposed an approximation to the XC functional that combines exact exchange, Spin Density Local Approximation (LSDA), and gradient corrections for XC. The proposed functional is applied to atoms and molecules, yielding a fit to experimental data with an accuracy of approximately 2 kcal/mol. Blöchl[51] formulated the Projector Augmented-Wave (PAW) method for calculating the electronic structure of solids, based on pseudopotential and Linear Augmented Plane Wave (LAPW) methods. The PAW method allows for a description of nuclei and valence electrons, avoiding pseudized potentials and is based on dividing space into atomic and interstitial regions, constructing projected wave functions that satisfy continuity and orthogonality conditions. Perdew *et al.*,[52] subsequently introduced a new Generalized Gradient Approximation (GGA-PBE) for XC

Table 3: Journals that publish on QDSCs, its impact factor and *h*-index according to Scimago and WoS (JCR) rankings.

Journal	WoS	Scopus	Impact Factor	H-Index	Quartile Scopus	Quartile Wos
Journal of Physical Chemistry C	5	22	1.03	323	Q1	Q2
Journal of Physical Chemistry Letters	4	9	1.85	235	Q1	Q2
Physical Chemistry Chemical Physics	2	9	0.82	272	Q1	Q1
Journal of the American Chemical Society	3	7	5.95	674	Q1	Q1
Nano Letters	1	8	3.54	531	Q1	Q1
ACS Nano	2	6	4.73	448	Q1	Q1
Journal Of Materials Chemistry A	0	7	3.16	270	Q1	Q1
Chemical Physics Letters	4	4	0.48	248	Q2	Q1
Chemistry of Materials	1	5	2.87	409	Q1	Q1
Advanced Functional Materials	2	4	5.57	376	Q1	Q1

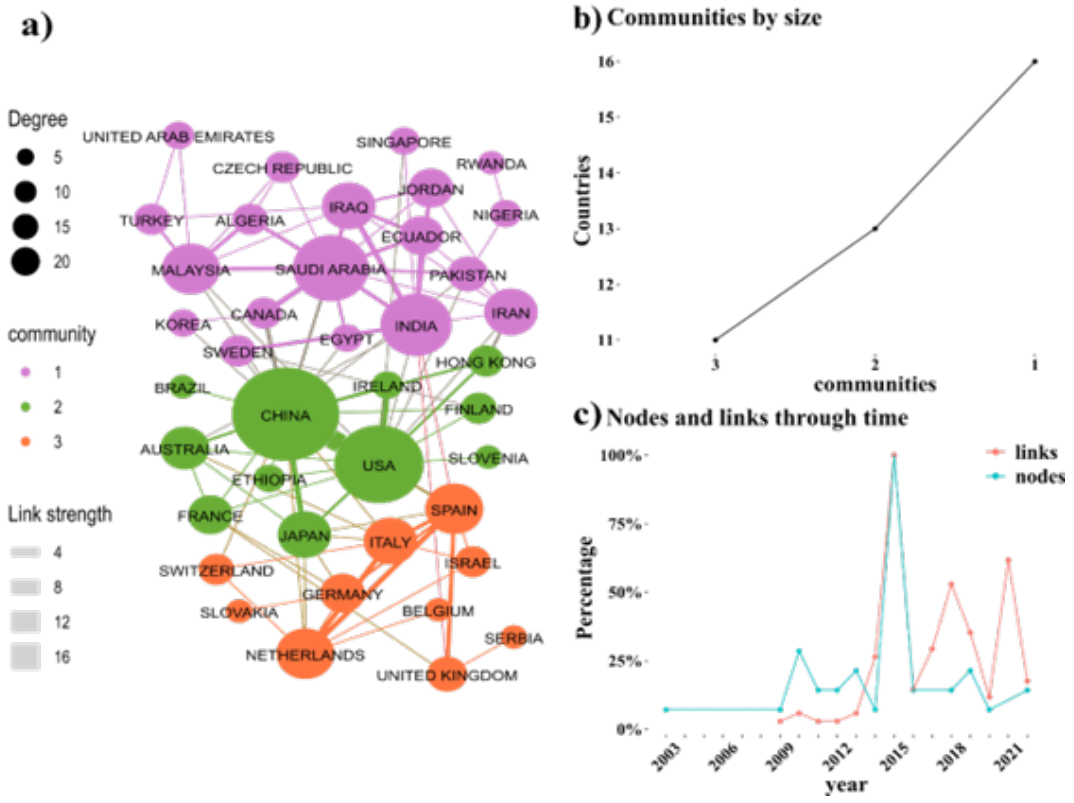

Figure 3: Scientific collaboration between countries a) network of countries, b) community by size and c) nodes and links over time.

Table 4: Total number of publications, Scopus *h*-index and affiliation of the most productive authors in QDSCs.

Sl. No.	Researcher	Total Articles*	Scopus *h*-index	Affiliation
1	Long R	10	45	Beijing Normal University, Beijing, China
2	Sarkar P	10	33	Visva-Bharati University, Santiniketan, India
3	Wang M	10	32	Ministry of Education of the People's Republic of China
4	Yang C	10	36	Ludong University, Yantai, China
5	Gao F	8	8	Hangzhou City University, Hangzhou, China
6	Ma X	8	29	Ludong University, Yantai, China
7	Infante I	7	48	Ikerbasque, Basque Foundation for Science, Bilbao, Spain
8	Li X	7	28	Harbin Institute of Technology, Harbin, China
9	Zhang L	7	70	Sichuan University Chengdu, China
10	Zhang Z	7	20	Fujian Normal University, Fuzhou, China

*Total articles is the sum of unique papers in WoS and Scopus.

energy. This approximation is simpler and more accurate than the Perdew-Wang 1991 (PW91) GGA.[53] The GGA-PBE improves upon several aspects, including a more accurate description of the linear response of the uniform electron gas and a smoother potential. The authors state that GGA-PBE produces comparable outcomes to PW91, but with a simpler form and derivation.

Kresse & Furthmüller[54] presented an efficient scheme for calculating the Kohn-Sham ground state of metallic systems using the pseudopotential method and a set of plane waves. The method is based on a self-consistency cycle, which divides the problem into matrix diagonalization and charge density mixing. The authors discuss various iterative algorithms for diagonalization. They also demonstrate that the number of iterations needed to achieve a specific accuracy is almost independent of the system size. Kresse & Joubert[55] established a formal relationship between Vanderbilt's ultrasoft pseudopotentials (USPP) and Blochl's PAW method. The authors presented a comparison of the accuracy and efficiency of PAW and USPP methods by linearizing two terms in a modified PAW total energy functional to obtain the total energy functional for ultrasoft pseudopotentials. Tao *et al.*,[56] proposed the non-empirical construction of a density functional for XC energy called meta-GGA. This functional includes electron density, its gradient, and Kohn-Sham orbital kinetic energy density. It is an objective and precise approach to calculating XC energy. Heyd *et al.*,[57] developed a density functional based on a screened Coulomb potential for exchange interaction to filter the long-range part of the Hartree-Fock exchange, retaining other unscreened Coulomb interactions. This enables more accurate and faster calculations, even in metallic systems. Despite significant progress in developing improved XC functionals for material description, the exact form of the ideal functional remains an open challenge.[58-60] However, ongoing research holds promise for the continued development of even more accurate functionals.[61] This ongoing pursuit of the optimal XC functional is often referred to as Jacob's ladder.[62-64]

Trunk

The trunk contains seminal works grounded in foundational research, paving the way for advancements in QDSC studies. Long & Prezhdo[65] investigated the dynamics of photo-induced Electron Transfer (ET) at the interface of a PbSe quantum dot and a TiO_2 surface. This process is crucial for enhancing QDSCs. The authors demonstrate that photo-induced ET at the PbSe-TiO_2 interface primarily occurs via an adiabatic mechanism due to strong donor-acceptor coupling. Ip *et al.*,[28] used DFT calculations to examine the electronic and optical properties of hybrid colloidal QDs passivated with various organic and inorganic ligands. The DFT results were compared with experimental data obtained through photoelectron spectroscopy and photoluminescence. Tan *et al.*,[66] studied the effect of hole-accepting ligands on the photo-stability of CdSe quantum dots, which are potential absorbers for QDs-sensitized solar cells. DFT calculations were utilized to estimate the ionization potentials of organic ligands bound to CdSe QDs using Koopmans' theorem. Additionally, the charge distribution in the molecule-surface complex was characterized using Natural Bond Orbital (NBO) analysis. In their study, Nadler & Sanz[67] investigated the impact of aliphatic and aromatic ligands on the optoelectronic properties of CdSe quantum dots using DFT. The study revealed that aromatic ligands have a greater impact on the optoelectronic properties of QDs compared to aliphatic ligands.

In a related study, Rimal *et al.*,[68] found that doping PbS quantum dots with manganese atoms resulted in a 300% increase in photocurrent. Ab initio calculations confirmed that the presence of Mn at the Pb quantum dot/Zn_2SnO_4 interface reduced the tunneling barrier height for electrons, which explains the observed increase in photovoltaic current. Rajbanshi & Sarkar[69] investigated the photovoltaic properties of CdTe quantum dot-porphyrin nanocomposites using the self-consistent charge density functional tight-binding method. The study focused on achieving type II band alignment in the

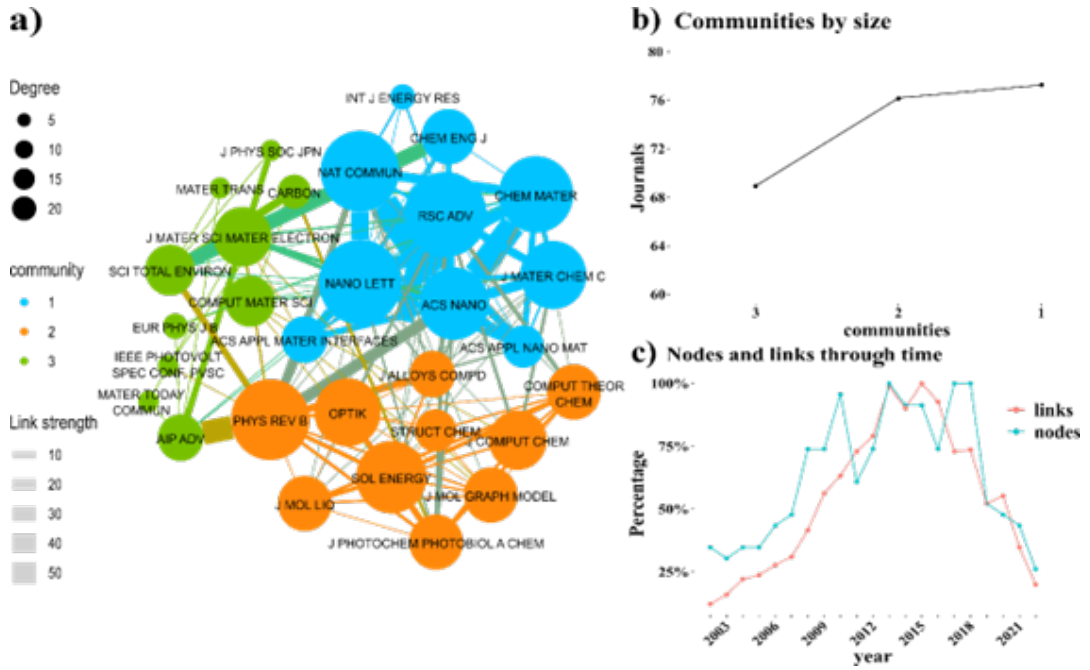

Figure 4: Journals where QDSCs topic are mainly published. a) journal network, b) communities by size and c) nodes and links through time.

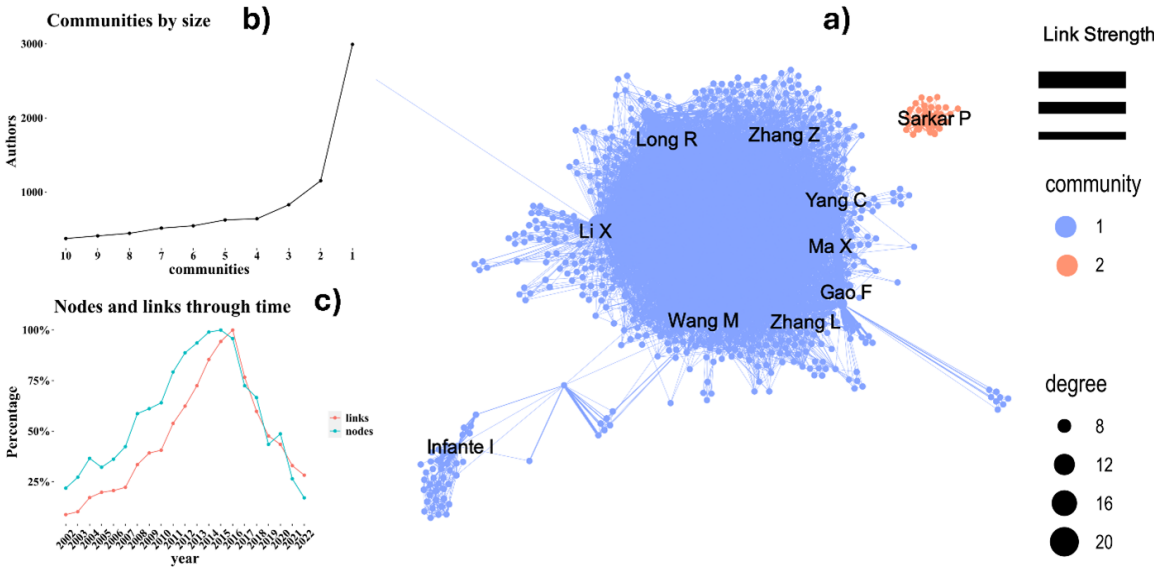

Figure 5: Scientific collaboration network between authors. a) authors' network, b) communities by size and c) nodes and links through time.

nanocomposites to enhance photovoltaic performance and avoid carrier recombination. Giberti *et al.*,[70] conducted a study on heterogeneous chalcogenide nanostructures with adjustable energy bandgaps under pressure. The study employed atomistic calculations to investigate how interfacial morphology and defects impact the electronic properties of PbSe and CdSe quantum dots. The study found that interfaces between PbSe quantum dots and CdSe matrices could generate harmful intra-gap states. Conversely, the reverse system (CdSe quantum dots in PbSe) exhibited superior electronic properties for photovoltaic applications. Additionally, applying pressure to the PbSe matrix was predicted to tune the CdSe structure and its energy bandgap.

In another study, Gao *et al.*,[71] investigated graphene QDs with Copper (Cu) metallized macrocycles using DFT. The optical absorption of optimized structures was calculated by the authors. It was noted that all QDs enhanced absorption in the

visible spectrum range. Sharma & Jha[72] investigated the effect of nitrogen (N), boron (B), and phosphorus (P) adatoms on carboxyl-functionalized graphene quantum dots (COOH-GQDs) for solar cell applications. The study showed that COOH-GQDs experienced a 22-30% increase in energy conversion efficiency after being doped with N, B, and P. These doped compounds are promising candidates for use in QDSCs applications.

The most recent research on solar cell efficiency can be divided into three branches (Figure 6). These investigations have led to the development of new materials and a better understanding of the mechanisms affecting solar cell efficiency, which has enabled their enhancement. A clear upward trend in QDSCs research is evident in Figure 7, with the slope of the data indicating a rapid growth in this field since 2010.

Branch 1 Halide Perovskites solar cells

Ray *et al.*,[73] investigated the charge transfer mechanism between $CsPbBr_3$ perovskite nanocrystals and Nitrogen-doped Carbon Quantum Dots (NCQDs) to form heterostructures with potential applications in optoelectronics and photocatalysis. The authors used DFT to calculate the electronic structure and charge density difference of the heterostructures to understand the charge transfer process. The study analyzes the impact of the thickness of the nanocrystal shell on carrier mobility and stability. This is crucial for applications such as solar cells and LEDs. Cai *et al.*,[74] investigated the use of graphene QDs modified with imidazole (IGQDs) in perovskite solar cells. The IGQDs improved energy conversion efficiency by passivating defects at the perovskite and tin dioxide (SnO_2) interface and accelerating carrier extraction and transfer. The authors reported an efficiency of 24.11% and high stability under ultraviolet irradiation. Nagal *et al.*,[75] investigated the slow cooling of hot carriers in $CsPbBr_3$ perovskite quantum dot-carbon nanolayer heterostructures. The authors studied charge transfer in the heterostructures through Ultrafast Transient Absorption Spectroscopy. Additionally, they performed DFT calculations to understand band alignment and confirm experimental results. Xu *et al.*,[76] investigated $CsPbI_3$ quantum dots with ligands to improve efficiency and perovskite film preparation. The authors reported an increase in grain size, a reduction in defects, a decrease in non-radiative recombination, and an improvement in charge transfer. The energy conversion

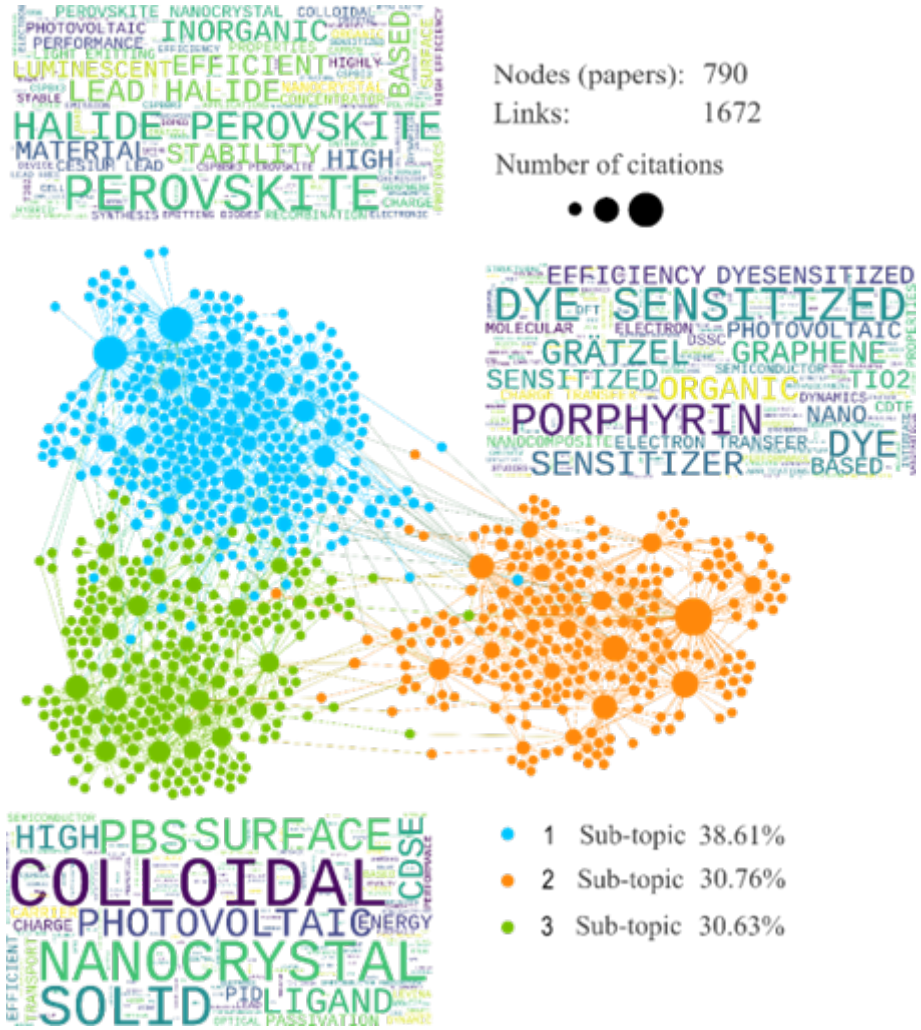

Figure 6: Networks and nodes of the main topics in QDSCs.

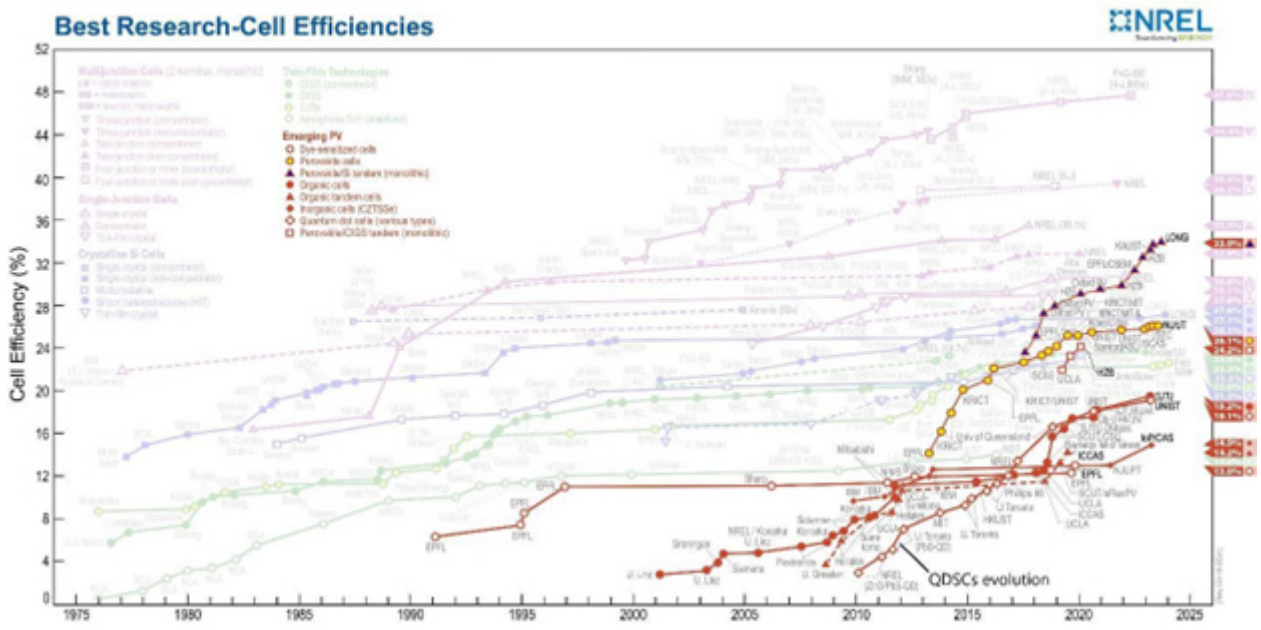

Figure 7: Evolution of best research-cell efficiencies for different technologies. Highlighted are the emerging photovoltaic technologies. QDSCs evolution is shown over time (2010-2023)

efficiency improved to 23.32%, surpassing that of the control device at 21.61%. The electronic structure of perovskite films under strain conditions was studied using DFT. Li *et al.*,[77] used DFT to investigate the electronic structure and optical properties of hexagonal Methylammonium Bismuth Iodide (MBI), employing the LDA-½ method and Spin-Orbit Coupling (SOC) effect. The predicted efficiency of MBI was 11.5%, which is 7 times higher than the experimental value of 1.64%,[78] indicating potential for the development of more efficient solar cells based on MBI. Pandey & Chakrabarti[79] investigated the optical and electronic properties of $CsPbI_3$ quantum dots using DFT and validated the results with experiments. The authors suggest that this material has significant potential for use in optoelectronics and solar cells.

Branch 2 Dye sensitized solar cells

Gao *et al.*,[71] conducted theoretical investigations on a nanocomposite consisting of Tetraphenylporphyrin (TPP) and Graphene Oxide Quantum Dots (GOQDs) as sensitizers in Dye-Sensitized Solar Cells (DSSCs). The authors used DFT to optimize geometric structures and Time-Dependent Density Functional Theory (TDDFT) to analyze optical absorption. Li *et al.*,[80] found that the GOQDs (18OH)-TPP compound shows potential as a sensitizer for DSSCs, providing insights for the development of solar energy capture materials. They also studied the optoelectronic properties of graphene-phenothiazine nanocomposites as a photoactive layer in solar cells using TDDFT. The authors reported that the combination of graphene and phenothiazine improved charge separation, light absorption, and light harvesting efficiency. This material shows promise for use in solar cells and optoelectronics. In a related study, Xing *et al.*,[81] investigated the use of nanocomposites of Phycocyanobilin (PCB) and Phycourobilin (PEB) with Graphene Quantum Dots (GQDs) as sensitizers in DSSCs. The geometric configurations were optimized using DFT, and stability was confirmed through vibrational frequency and formation energy analysis. The electronic properties of the GQD2-PEB nanocomposite suggest its potential as a favorable sensitizer due to apparent charge spatial separation, appropriate frontier orbital energies, and enhanced absorption coefficient in the solar irradiation region. Majid *et al.*,[82] used TDDFT to model photon injection in organic dye/TiO_2 systems. Their aim was to explore enhancements in Dye-Sensitized Solar Cells (DSSCs). The authors proposed structural modifications in carbazole-based organic dyes by altering the π-bridge and introducing thiophene and oxadiazole rings. These modifications affected the optical and electronic properties. Jain *et al.*,[83] studied the optical and electronic properties of CdS quantum dots sensitized with dyes. They observed a significant distortion in the quantum dot structure when strongly interacting with the dye. The position of the energy levels of the dye and the QDs varies depending on the configuration. In their investigation the use of TiO_2 Electron Transport Layers (ELTs) in Sb_2Se_3 solar cells, Don *et al.*,[84] aimed to replace toxic CdS ETLs. By optimizing TiO_2 processing conditions, the research achieved a power conversion efficiency of 8.12%, highlighting the potential for more efficient and environmentally friendly solar cells.

Branch 3 Nanocrystal solar cells

Kumakura *et al.*,[85] calculated the temperature-dependent carrier mobility and optical properties of lead sulfide Quantum Dots (PbS QDs) with Formamidinium (FAI) and Chlorine (Cl) ligands using DFT and Non-Equilibrium Green's Function

(NEGF) techniques. The authors reported that QDs with Folic Acid (FA) ligands exhibit higher mobility and enhanced optical absorption compared to those with Cl ligands. This is attributed to the intermediate band electronic structure that influences transport properties. These findings suggest that FA ligands could be more efficient for solar cell applications due to their higher mobility and optical absorption. This marks a promising step toward the development of more efficient low-dimensional optoelectronic devices. Yazdani *et al.*,[86] aimed to comprehend the transport, generation, and trapping of charge carriers in semiconductor-based nanocrystal QDs through DFT simulations. The DFT results were used to create a predictive model to understand how the presence of a charge carrier in an individual quantum dot can lead to polaron formation, which is crucial for the charge transport mechanism in these systems.

Fuhr *et al.*,[87] investigated the impact of anti-site defects and copper vacancies in $Cu_xIn_{2-x}S_y$ quantum dots (QDs-CIS) on their optical properties, which are essential for energy harvesting applications. The authors utilized DFT calculations to predict the effects of different defects on optical spectra, consolidating various proposed emission models. The authors state that the study enhances the performance of devices such as solar cells and Luminescent Solar Concentrators (LSCs) by providing a clearer understanding of structure-property relationships in QDs-CIS. Oh *et al.*,[88] conducted research on Silver Bismuth Sulfide Nanocrystals ($AgBiS_2$) for thin-film photovoltaics. The chemical composition and crystal structure of the nanocrystals were revealed through X-ray Photoelectron Spectroscopy (XPS) and X-ray Diffraction (XRD) analyses. To determine the stability of iodine ligands after water treatment, DFT was used to calculate the binding energies of iodine on various $AgBiS_2$ and PbS surfaces. DFT calculations have facilitated a more profound comprehension of chemical interactions on nanocrystal surfaces and their water resistance. This is crucial for the development of stable, lead-free photovoltaic materials.

Singh *et al.*,[89] conducted DFT calculations to investigate the stability and electronic properties of single-walled Si_2BN nanotubes. Their study confirmed the structural stability of these nanotubes and explored the impact of rolling Si_2BN sheets into nanotubes on chemical bonding and conductivity. The research highlights the unique properties of Si_2BN nanotubes, and their potential applications in electronic and materials science.

CONCLUSION

This study compiled publications related to QDSCs using DFT, classifying 278 consolidated references from Scopus and WoS databases. Two analyses were conducted: a scientometric analysis and one using the ToS algorithm. The study identified changes and the impact of scientific production over the past 22 years, enabling researchers to identify important contributions in the field of QDSC research. The analysis highlights a significant increase in DFT-based research on QDSCs, particularly from 2012 to 2019, with a growth rate of 38.95%. This growth is driven by studies focusing on QDs and graphene to enhance solar cell performance using DFT simulations. The increasing number of Scopus and WoS indexed publications highlights DFT's growing importance as a computational method tool for understanding and optimizing QDSCs. This trend reflects a rising interest in using advanced computational methods to optimize solar cell technologies.

The study reveals that China leads in the number of publications with 71 articles, followed by the United States with 46 articles. However, the citation impact is nearly comparable, with the USA at 26.23% and China 30.21%. This indicates that while China is producing more research, the USA's contributions remain highly influential, suggesting a competitive landscape in QDSC research. In terms of journals, the findings show that the Journal of Physical Chemistry C has the highest production, with 22 publications in Scopus and 5 in WoS, with a significant number of publications in high-impact journals (nine out of ten in Q1). This underscores the high quality of research in this field and suggests that findings from these journals are likely to influence future studies and applications in solar technology.

The analysis of scientific collaboration networks indicates a high level of cohesion, despite limited collaboration among the most productive researchers.

Although this study did not explore technical aspects and only selected representative research, it still provides valuable insights for researchers interested in studying QDSCs using DFT. Given the significant growth in QDSC research over the past three years, future research should focus on interdisciplinary approaches that combine experimental and computational techniques to optimize the efficiency and practical applications of QDSCs.

DFT has proven to be an important computational method for understanding the electronic properties and stability of materials used in QDSCs. DFT calculations can be used to design new materials with specific properties, potentially leading to a significant improvement in solar cell efficiency.

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CONFLICT OF INTEREST

The authors have no competing interests to declare that are relevant to the content of this article.

AUTHOR CONTRIBUTIONS

I. Arellano-Ramírez: Conceptualization; Formal analysis and investigation; Writing – original draft. L. Bohorquez Santiago: Methodology; Data curation. A. Gil Rebaza: Writing – review and editing, supervision. S. Amaya-Roncancio: Writing – review and editing, supervision. E. Restrepo-Parra: Supervision and Funding acquisition.

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