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Review paper

Application of Machine Learning Algorithms in Improving Nano-based Solar Cell Technology

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Abstract

This study explores the potential use of Machine Learning (ML) techniques to enhance three types of nano-based solar cells. Perovskites of methylammonium-free formamidinium (FA) and mixed cation-based cells exhibit a boosted efficiency when employing ML techniques. Moreover, ML methods are utilized to identify optimal donor complexes, high blind temperature materials, and to advance the thermodynamic stability of perovskites. Another significant application of ML in dye-sensitized solar cells (DSSCs) is the detection of novel dyes, solvents, and molecules for improving the efficiency and performance of solar cells. Some of these materials have increased cell efficiency, short-circuit current, and light absorption by more than 20%. ML algorithms to fine-tune network and plasmonic field bandwidths improve the efficiency and light absorption of surface plasmonic resonance (SPR) solar cells. This study outlines the potential of ML techniques to optimize and improve the development of nano-based solar cells, leading to promising results for the field of solar energy generation and supporting the demand for sustainable and dependable energy.

1. Introduction

In the recent years, human population growth has increased at an accelerated rate, and it is estimated that the global population will surpass 8.6 billion by 2030 and 9.8 billion by 2050 [1]. At present, the primary source of energy for human consumption is derived from fossil fuels including oil, coal, and natural gas [2]. However, the utilization of these finite resources is responsible for significant and irreversible environmental impacts. The exploitation of renewable resources represents an opportunity for a paradigm shift in global energy supply, while ensuring environmental sustainability. Solar energy is one of the most prevalent forms of renewable energy sources employed at present, and holds considerable promise for the future [3,4]. The most prevalent technology utilized for harnessing solar energy is through the use of solar cells, which are capable of generating electricity directly from sunlight. The high cost and the complicated manufacturing technology of older solar cells have led to research into newer types of solar cells. As a result, the development of second-generation thin-film solar cells through the utilization of nanoscience has been pursued [5]. These solar cells have advanced significantly in the recent years, and the employment of nanoscience has substantially improved their productivity [6]. Nanoscience has permitted advancements in the design and fabrication of second-generation thin-film photovoltaic cells (PVs). It has also enabled the scientists and manufacturers to create more efficient solar cells utilizing cheaper materials such as silicon and titanium dioxide (TiO_2) [7].

Machine Learning (ML) has been a popular area of research in the recent years. It enables computers to process databases and enhance future project predictions through the utilization of historical data [8, 9]. The employment of ML

in many laborious and expensive projects results in cost reduction, time-saving, and increased work efficiency. In addition, machines enhance accuracy while eliminating or reducing human error [10]. ML can also be utilized to solve problems that possess uncertain rules influenced by variables engineers cannot effectively code [11]. Due to the advancements in computing technology, ML has been widely implemented in various domains, particularly in the context of solar cells. It has demonstrated significant improvement to various aspects of solar cell technology. A thorough comprehension of these applications can be attained by referring to numerous review articles recently published in this field. These publications cover extensive research regarding solar cells' new materials that have been discovered by employing ML techniques [10,13]. Additionally, many of these sources provide information on other applications involving improved efficiency, optimization of solar cells, and other related topics [13,15].

In the recent years, substantial research has been conducted regarding the intersection of solar cells and ML. Li et al. [18] published a comprehensive study in 2019 that examined ML's potential applications across various types of solar cells. Within the paper, the primary solar cell applications of ML were categorized into four distinct groups, which encompassed material property prediction, device structure optimization, manufacturing process optimization, and measurement data reconstruction. The researchers ascertained that the artificial neural network (ANN) and genetic algorithm (GA) implementations were the most well-suited algorithms for solar cells. Due to the inherent uncertainty of solar energy, several review articles have been published that explore the ML approach in solar cell power prediction [16,17], solar irradiance prediction [16,19], and identifying the optimal power point of solar cells [16].

Due to the rapid advancements in nano-based solar cells, numerous review articles have emerged that examine ML's applications for particular types of nano-based solar cells. In the context of perovskite solar cells (PSCs), the majority of ML applications focused on material search and improvement. In 2021, Yılmaz and Yıldırım [17] conducted a literature review of research on new materials discovered for PSCs utilizing ML techniques. The outcomes of this review indicated that, in addition to the benefits of cost reduction and increased efficiency of scientific evaluations, the use of ML may result in issues such as an increase in the quantity of unreliable models and research models with inadequate validation. Zhang et al. [14] similarly investigated the potential for ML to discover new halide PSC materials such as lead-free, stable materials. Via ML-based tools, the researchers identified promising structural and contextual predictive relationships and materials, including cap additives. Their discoveries demonstrate how ML may facilitate structural-property connection identification and substance identification, thus contributing to materials science's simplification and optimization.

The utilization of ML for dye-sensitized solar cells (DSSCs) has predominantly been for discovering more efficient dyes and enhancing the overall operation of these cells. In a study conducted by Michaels et al. [23], advanced materials suitable for solar cells – notably DSSCs – were examined. This research work also explored the potential impact and application of these cells in the development of next-generation internet of things (IoT) technologies. Ju et al. [15] investigated the efficacy of data mining methods in conjunction with quantum chemical methodologies to probe the effectiveness of new N-annulated perylene sensitizers in DSSCs. The findings delineated that these novel materials provide advantages such as increased efficiency, improved charge transfer, and enhanced optoelectronic properties in comparison to older materials.

Manzhos et al. [24] conducted an examination of recent literature to acquaint themselves with the latest approaches concerning nanoplasmonics modeling in solar cells. Based on their findings, it is anticipated that the use of functional tight-binding (DFTB) approaches, time-dependent orbital-free approaches (DFT), ML techniques, and many-body perturbation theory approaches will expand as computational power continues to evolve. In specific considerations, some research works utilize ML techniques to enhance the light absorption of Surface Plasmonic Resonance (SPR) solar cells [25], increase plasmonic field bandwidth to optimize the absorption of the visible light spectrum [26] , and determine the optimal layer thickness [27]. These studies comprise a subset of those that have relied upon ML in nanoplasmonic research, which continues to offer an avenue of exploration for novel methodologies and optimizations for solar cells.

This research has investigated the implementation of ML approaches in the context of three different categories of nano-based solar cells: PSCs, DSSCs, and SPR solar cells. The primary rationale for selecting nano-based solar cells as

the central focus of this study is their intimate relationship with nano-science, which exerts a significant influence on enhancing solar cell conversion efficiency, in addition to their contributions towards introducing and refining second-generation solar cells. Furthermore, utilizing more cost-effective, and widespread materials in solar cells fabrication adds an additional reason for the importance of nano-based solar cells in this study.

PSCs hold considerable relevance in the field of solar cells, and recent years have seen significant advances in PSC research. They possess the ability to assimilate diverse light wavelengths, leading to advanced operating efficiencies [28]. Additionally, the inherent rise in light assimilation in these cells has brought about a significant reduction in the perovskite material employed, culminating in substantial decreases in the cost of manufacturing and the eventual market value of these cells [29]. Furthermore, certain characteristics of perovskites, such as their light weight, semi-transparency, pliability, and tailor-made form factor, have played an elevated role in enhancing their relevance in the context of solar cells.

DSSCs constitute another category of solar cells that are analyzed here. The functional mechanism of these cells relies upon natural sensitizers. Factors that have augmented their relevance in solar cells include the inexpensiveness engendered via the use of low-cost raw materials [27,28], manufacturing and processing simplicity [28], and exclusively non-toxic exposure [32]. Additionally, transparency and reasonable performance [28], coupled with the high adaptability to normal radiation and cloudy weather conditions [33], elevate their superiority over other solar cells.

The last classification of nano-based solar cells contemplated in this investigation is the SPR solar cells. The application of SPR technology spans numerous domains. As a real-time, label-free, and non-invasive methodology, SPR has been conferred significance within the realms of biochemistry, biology, optical biosensing, and medicine [34]. The primary rationale for the prevalence of SPR within the context of solar cells stems from its efficacy in augmenting the absorption of light, which contributes to an increase in solar cell efficiency.

The objective of this study is to examine the effects and enhancements of PSCs, DSSCs, and SPR solar cells utilizing ML algorithms. As previously noted, some review articles have partially explored the application of ML to certain nano-based solar cell patterns. However, the scope of these articles was generally geared towards discovering new materials for these cells. Conversely, this comprehensive review has analyzed all potential ML applications published in recent articles. In the instance of PSCs, investigation into the discovery of new materials, deposition methods, stability, and other related aspects were also conducted. With regard to DSSCs, ML methods were employed to develop perylene sensitizers, discover new molecules for DSSCs, and predict the efficiency of organic DSSCs, in addition to examining the different layers of DSSCs, including the electrodes, TiO_2 layer, and electrolyte, to optimize performance. Furthermore, various optimization techniques were studied in SPR solar cells to ameliorate light absorption, increase efficiency, and optimize cell layer thickness. One of the key strengths of this study lies in its all-inclusive investigation into the three types of nano-based solar cells, i.e., perovskites, DSSCs, and SPR solar cells, with respect to ML applications, which enables the precise identification and comparison of these applications in each solar cell category. This research can facilitate expeditious identification of problems that can be resolved through ML and suggest more rapid and cost-efficient approaches to enhance and optimize solar cell performance. Accordingly, this review collected recently published articles in various journals that optimized and incorporated artificial intelligence algorithms in PSC, DSSC, and SPR solar cells. Furthermore, an in-depth scrutiny of the exact application of such algorithms in these works was performed. Ultimately, the research results emphasized the fundamental challenges inherent in these solar cells which can be resolved and improved through ML.

2. Methods and Materials

2.1. Perovskite solar cells

Apart from other noteworthy applications, nanotechnology has made significant strides in the context of solar cells, with PSCs constituting one such application. The foundation for this cell was initially established by Miyakasa et al. [35]. Functionally, a PSC operates similarly to a pin diode, with its active perovskite layer serving as a conducting semiconductor, and the cavity and electron transfer layers being categorized as P and N layers, correspondingly. The metallization layer operates as an access electrode. The cells function by utilizing the electric field generated by electron pairs, which produce a separation of holes, resulting in the migration of electrons towards the

electron transport layers (ETL layer), and holes towards the hole transport layer (HTL layer), ultimately terminating at the specified electrodes [36]. Figure 1 provides an illustration of the layer-by-layer structure of a PSC.

The stability of PSCs is contingent on environmental circumstances, including variables such as humidity and oxygen [34,35], temperature [39], applied potential [40], ultraviolet light [41], visible light [42], and fragility [43]. Figure 2 represents the progression of PSCs efficiency over the course of the year 2020.

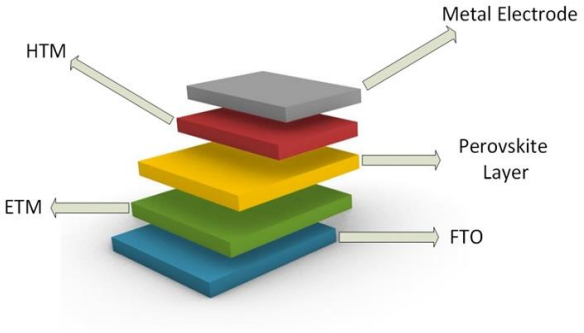


Figure 1. Various layers of a PSC (based on the data from reference [44]**).**

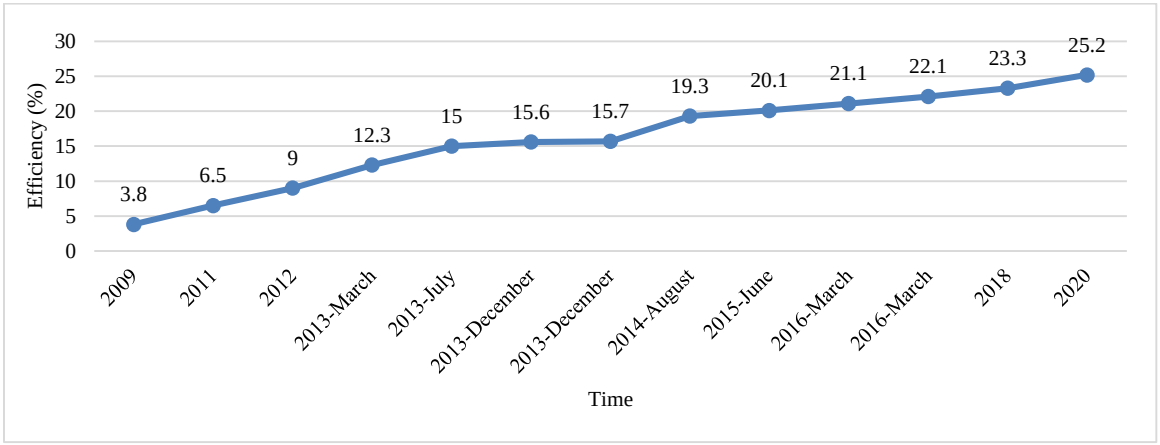


Figure 2. Increase in the efficiency of PSCs (based on the data from reference [45]**).**

2.2. Dye-sensitized solar cells

DSSCs are categorized as part of the thin-film solar cell cohort [46], first developed by Brian O'Regan and Michael Graetzel in 1988 [47]. As compared to other types of thin-film cells, DSSCs exhibit lower efficiency rates. The core constituents of a DSSC entail a top-side anode consisting of fluorine-doped tin oxide (SnO2: F), a subsequent sub-layer of TiO_2, and finally, placement within a photosensitive ruthenium polypyridyl solution [48]. As evidenced by existing research, the efficiency of these cells ranges between 11% [44,45] and 15% [30,46], signifying their relatively lower performance in contrast to other cell types. However, the preliminary nature of these cells has invited extensive exploration, indicating a potential for refining performance. In this regard, ML comprises an essential component with the potential to augment the effectiveness of DSSCs by devising new materials and dyes and optimizing the various layers integral to these solar cells, including the electrode, electrolyte, and TiO_2 counterpart. Figure 3 depicts the contrasting structure of a thin-film DSSC and its mechanism of operation.

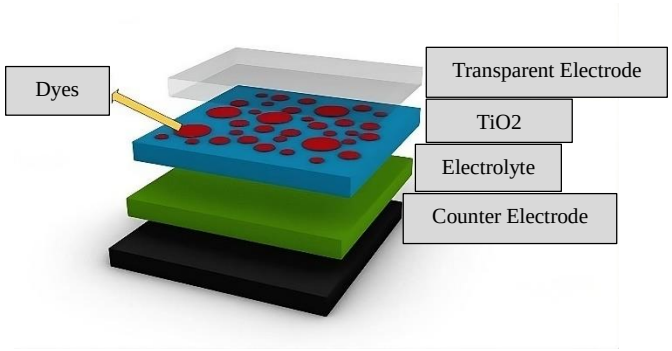


Figure 3. Structure of a DSSC (based on the data from reference [52]**).**

2.3. Surface plasmonic resonance solar cell

SPR is the resonance that occurs between conduction electrons at the interface of materials with positive and negative transmission coefficients, which is stimulated by light [53]. Surface plasmon polariton features a non-radiative surface electromagnetic wave that propagates parallel to the interface between neg
ative permittivity coefficient and dielectric material. Since these oscillations transpire at the boundary between conductors and external mediums, the movement of these waves manifests

great sensitivity to boundary changes like the adsorption of molecules on the conducting surface [54]. SPR is established when an incident light photon strikes a metal surface such as a gold surface. Under a specific incidence angle, some of the light energy couples with electrons in the metal surface layer via the metallic coating and moves due to the excitation. These plasmons possess the capacity to generate a 300 nm electric field between the metal surface and the sample solution [55]. The range of applications for plasmons encompasses Raman scattering with escalated surface area [56] and bio-optical sensors [57]. Notably, plasmonic enhancement applied through surface dispersion on noble metal constitutes a prime method for increasing light absorption, a critical factor in the effectiveness of solar cells [58]. Enhancing absorption boosts the short-circuit current (Isc) and cell efficiency [59]. In 2018, researchers delved into the impact of SPRs on nanoscale gold particles. Their findings illustrated that light absorption grows linearly in relation to nanorod concentration. In the optimal scenario, overall efficiency in Y123-sensitive cells rises by roughly 66% (from 5.31 to 8.86%) [60]. Figure 4 presents an overview of the working principle of an SPR solar cell.

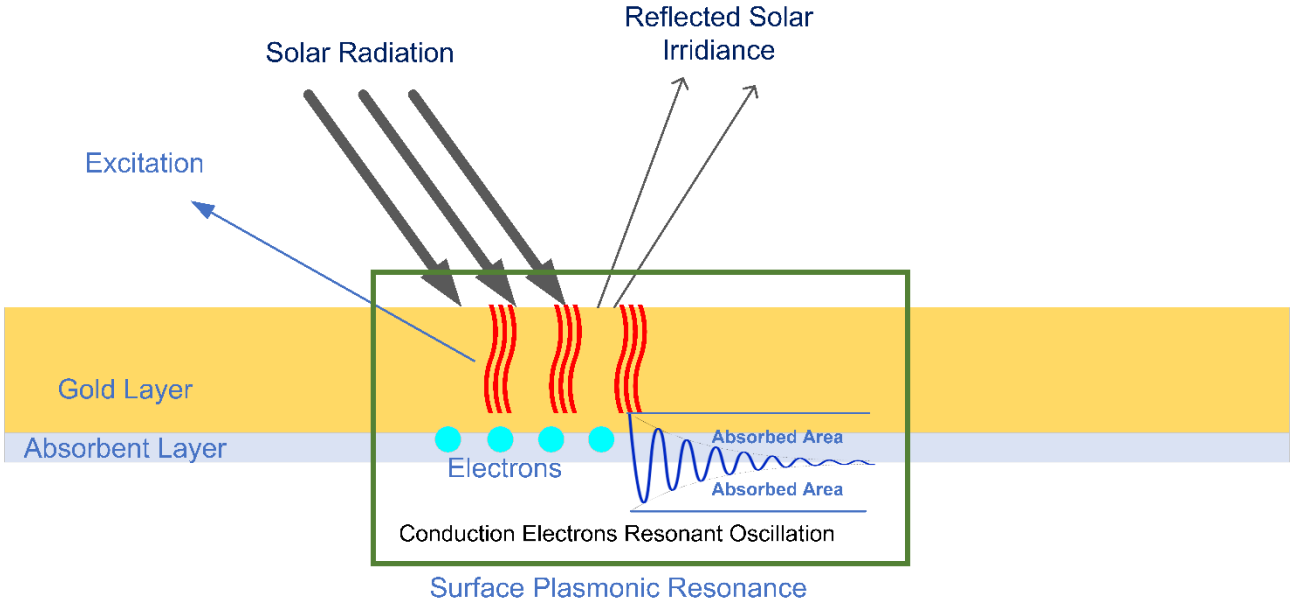


Figure 4. How to trap and increase light absorption in SPR solar cells (based on the data from reference [61]**).**

2.4. ML

Today, many researchers are extensively focusing on enhancing the structure of introduced cells, with ML and related algorithms amongst the relatively modern, efficient, and widely utilized approaches within this research domain. The origin of ML can be traced to the 1950s, beginning with the inception of the first neural network [62], as initially devised by Arthur Samuel in 1959 for computer games and artificial intelligence purposes [57,58]. The classification of information, and the subsequent prediction of future outcomes based upon the acquired data constitutes the fundamental strategy utilized in ML research [65]. In achieving categorized information, particular types of algorithms are applied. Some of the prevalent algorithms employed in ML incorporate the ANN [66], GA [67], Particle Swarm Optimization (PSO) [62,63], Random Forest (RF) [70], and so on. A significant proportion of these algorithms finds their origins in nature. For instance, ANN traces its inspiration to animal brains [71], whereas GA prides itself on replicating the phenomenon of natural selection [72]. In the case of PSO, the algorithm draws inspiration from the mathematical formula used to calculate the movement of particles towards the optimum position [73].

The employment of ML for solar cells has seen significant advancements. The applications of ML in solar cells can be broadly classified into four categories, namely material property prediction, structural optimization, manufacturing process optimization, and measurement data reconstruction [18]. Even though in recent years, the majority of ML applications in nano-based solar cells have been directed towards finding novel materials for varying solar cell types, this study endeavors to examine all areas in which ML may facilitate the development and optimization of nano-based solar cells, including PSC, DSSC, and SPR cell. These investigations will

concurrently address all three cell types, thereby enabling the identification and comparison of challenges across said cell types, followed by the application of ML methodologies towards confronting these challenges. To this end, we will initially describe the utilized ML algorithms subsequently followed by an overview of the existing literature available on the aforementioned cell types.

3. Challenges of solar nano-based solar cells

In prior sections, a selection of articles on nano-based solar cells including PSCs, DSSCs, and SPR solar cells have been presented. This section aims to review the aforementioned articles in addition to the research conducted in previous sections concerning the primary challenges presented by these cells, specifically, those conquerable by means of ML. Efficiency remains one of the main obstacles faced by all three cell types examined. Despite marked enhancements in solar cell efficiency throughout recent years, potential for progressive advancements persist. ML, by analyzing a range of compounds, and their impacts on solar cells, can aid in the development of novel materials, in turn leading to significant enhancements in cell efficiency.

One of the challenges associated with PSCs is their insufficient stability for practical applications. Therefore, a substantial amount of research is required to develop innovative compounds and enhance their stability. ML can be a powerful tool to address this issue by facilitating the discovery of new materials and optimization of the cell structures. Moreover, significant efforts have been made towards the development of lead-free PSCs, as reported in several articles.

The structural optimization of nano-based solar cells is one of the primary challenges that researchers encounter. Altering cell parameters such as material thickness or concentration can improve cell function. These optimizations are mainly performed using ML algorithms.

One of the issues associated with SPR cells is the light absorption problem. One of the major challenges is to increase the light absorption in these cells. The solution to this challenge can be achieved by either structurally optimizing the cells or introducing new metal nanoparticles.

4. Applications of ML in Nano-based Solar Cells

In this section, we will explore the applications of ML in advancing and improving the performance of nano-based solar cells. In this regard, we present several articles that address the use of ML algorithms in the area of PSCs, DSSCs, and SPR solar cells. We will review the findings of these studies to highlight the outcomes of applying ML techniques to enhance the performance of these types of solar cells.

4.1. Application of ML in PSCs

ML is widely recognized as an invaluable tool for the advancement of PSCs. Various applications of ML have been applied to enhance the understanding and development of PSCs including predicting material properties, introducing novel materials, exploring cell stability, and estimating cell efficiency. In this study, the applications of ML in PSCs are categorized into three primary domains: materials selection, construction process optimization, and material property prediction. Recent studies are then highlighted within each category, and their collective findings are presented as follows.

4.1.1. Selecting proper materials

In 2018, Ozer and Yildirim [74] examined a database of 1921 records from over 800 lead halide PSCs. This research aimed to develop ML models for predicting cell performance. The study employed association rule mining, decision tree classification, and RF regression as the chosen techniques. The results of this work indicate the incorporation of novel materials in various components of the cells. Table 1 displays a selection of variables utilized (pertaining to the selection of new materials), and the energy conversion efficiency was also considered as a key metric.

After applying the algorithms, it was concluded that the efficiency of the cells is almost the same in the case of Methylammonium lead tri-iodide (MAPbI3) and MAPbI3-xClx. FA and mixed cation-based cells have higher efficiencies. Some features like mixed cation perovskites, Dimethylformamide (DMF) + Dimethyl sulfoxide (DMSO) as a solvent, and chlorobenzene as solvent are also effective in achieving efficiencies above 18%. Less common compounds such as lithium bis(trifluoromethane)sulfonimide (LiTFSI) + 4-tert-butylpyridine (TBP) + tris[4-(tert-butyl)-2-(1H-pyrazol-1-yl)pyridine]cobalt(II) bis(trifluoromethanesulfonimide) (FK209) as HTL additive and SnO_2 as ETL layer were also identified as options for high yield cells. The use of poly[bis(4-phenyl)(2,4,6-trimethylphenyl) amine (PTAA) as HTL, mixed cation perovskite, and bathocuproine (BCP) as ETL layer were also found to be important parameters for high efficiency in reverse cells [74].

In 2018, Lou et al. [75] proposed a method to detect materials used in organic and inorganic PSCs by combining ML with functional density theory. Several algorithms were used in this research. Based on the three criteria of coefficient of determination (R2), Pearson coefficient, and mean square error (MSE), the gradient boosting algorithm (GBR) was identified as the appropriate algorithm. Fourteen important features were analyzed, and their results are presented in Table 2. Table 2 shows the importance of each feature. According to this table, the most important features are T_f (tolerance factor), IC_B (total number of ionic charges), O_f (octahedral factor), respectively. According to the predicted results, the optimal tolerance factor was between 0.8 and 1.2, and the octahedral factor should be between 0.4 and 0.7. After removing insignificant features and considering the most important features, six candidate materials were selected using density functional theory (DFT) and ML calculations. The tolerance factor and octahedral factor for these six materials ranged from 0.82 - 1.04 and 0.5 - 0.57, respectively.

In 2020, Odabaşı and Yıldırım [76] conducted a study on the effects of various features and materials on the stability of PSCs. In their research, they employed ML techniques such as decision trees and association rule mining, utilizing a dataset consisting of 404 organolead halide perovskites. The findings of their study provided recommendations for the selection of suitable materials for different components of PSCs. Table 3 presents these materials and their respective applications.

Table 1. Related variables to new material selection used in research (power conversion efficiency has been considered as output) (based on the data from reference [74]**).**

Factor	*Alternative*	*Results*
Perovskite type	MAPbI3, MAPbBr3, MAPbBr3-xClx, MAPbI3-xBrx, MAPbI3-xClx, MASn1-xPbxI3, FA based, Cs based, Sn-based, mixed cation, mixed halide perovskites [MA=CH3NH3, FA=CH[NH2]2]	MAPbI3 and MAPbI3-xClx have the same performance. Also FA and mixed cation-based cells have better performance.
Precursor solution	DMF, DMA, DMF+DMSO, DMF+CHP, DMF+DIO, DMF+GBL, DMF+H3P, DMF+HI, DMSO, DMSO+GBL, DMSO+SnF2, GBL, 2-methoxyethanol+CHP	DMF+DMSO as solvent was effective to reach higher efficiencies.
Anti-solvent treatment	chlorobenzene, toluene, diethyl ether, trifluoro toluene, ethyl acetate, ethanol, without anti-solvent treatment	Chlorobenzene was a candidate to increase the performance
ETL	**Regular:** *[as compact layer]* C60, SnO_2, TiO_2, TiO_2-doped, ZnO, ZnO-doped, Fe_2O_3, graphene, PCBM, without ETL **Inverted:** PCBM, doped PCBM, C60, PCBM+C60, ZnO, without ETL	SnO_2 was detected as a candidate for higher efficiencies.
HTL	**Regular:** spiro-OMeTAD, CuSCN, P3HT, PEDOT, PTAA, SWNT, without HTL **Inverted:** PEDOT: PSS, PEDOT: PSS-doped, CuSCN, GO, NiOx, doped NiOx, PTAA, without HTL	PTAA as HTL in inverted cells helped to reach higher efficiency.
HTL additive *[for regular cells only]*	LiTFSI+TBP, LiTFSI+TBP+FK102, LiTFSI +TBP+FK209, LiTFSI, LiTFSI +2,6lutidine, without additive	LiTFSI+TBP+FK209 as HTL additive helped to reach higher performance.

Table 2. Importance and correlation of selected features using the GBR algorithm (based on the data from reference [75]**).**

Factor	Importance (%)	*Factor*	Importance (%)
T_f	23.8	EA_B	4.9
IC_B	16	P_B	4
O_f	12.6	r_B^{s+p}	3.7
$X_{p\text{-}electron}$	7	$HOMO_A$	3.1
P_A	6.9	r_A	2.1
IE_B	6	r_B	2.1
X_B	5.9	$LUMO_A$	1.9

Table 3. New materials and their application in various parts of the PSCs to reach better stability (based on the data from reference [76]**).**

Materials	*Application*
mixed cation perovskites	-
DMF + DMSO	precursor solution
chlorobenzene	anti-solvent
SnO2	ETL
PCBM	Second ETL
LiTFSI + TBP + FK209 and F4TCNQ	HTL additives
Carbon	Back contact
PTAA and NiOx	HTL
PCBM + C60	ETL ,BCP interlayer

4.1.2. Optimization of construction process

Another application of ML in PSCs is the optimization of the construction process, which has been mentioned in recent studies. For instance, Ozer and Yildirim [74] conducted a comprehensive analysis of a database consisting of 1921 records, suggesting methods to enhance the construction process while also identifying novel materials. Table 4 presents the alternatives proposed in their research for optimizing the construction process. The results demonstrated that the two-stage deposition method yielded higher efficiency. However, in recent years, the single-stage method has emerged as superior, primarily attributed to advancements in solvents and antisolvents. Additionally, applying double or triple rotation as a single-stage coating may prove instrumental in achieving higher efficiencies (exceeding 18%).

Table 4. New materials and their application in various parts of the PSCs to reach better stability (based on the data from reference [76]**).**

Factor	*Alternative*	*Results*
Perovskite deposition procedure	one-step, two-step	Two-step deposition resulted in better performance
Perovskite deposition method	spin, spin 2-3, spin-dip, spin 2-3-dip, dip coating, VASP, CVD, evaporation-spin, spin-spray, spray, spin-dripping	2- or 3-times spinning was a way to improve cells performance
The second layer of ETL/ETL interlayer [ETL-2]	**Regular:** C60, PCBM, $mTiO_2$, doped $mTiO_2$, mAl_2O_3, TiO2-ns, ZnO-ns, without ETL-2 layer [m-mesoporous, ns-nanostructure] **Inverted:** ZnO, TiOx, PEI, LiF, Ca, Bphen, BCP, Ba, AZO	BCP as ETL layer in inverted cells was a significant factor for cells efficiency.

In 2019, Chen et al. [77] employed ML to detect crystal grains in the perovskite layer. The control of the crystallization process is deemed challenging in the fabrication process due to the poor morphology of the perovskite layer. The study's results demonstrate the potential use of scanning electron microscope (SEM) images for analyzing perovskite crystals, with potential application to other types of PV devices like thin-film cells that also necessitate crystal analysis. Moreover, this approach can save a significant amount of time typically spent on manual crystal analysis. In 2020, Odabaşı and Yıldırım [78] tried to investigate the hysteresis and reproducibility of PSCs and their relationship relation with cell features using ML. They used two datasets containing more than 600 published results. According to their results, some features such as two-step spin coating or multiple spin coating in one step and some materials such as dimethylformamide + dimethyl sulfoxide as precursor solution, poly bis[4-phenyl][2,4,6-trimethylphenyl]amine as hole transport layer (HTL),Lithiumbis[trifluoromethanesulfonyl]imide + 4-tert-butyl pyridine + tris[2-[1H-pyrazole-1-

yl]-4-tert-butyl pyridine] cobalt[III] as HTL dopant may be important significant due to their having high reproducibility and low hysteresis. Moreover, these properties have a great impact on efficiency and stability. In a study conducted in 2020, Odabaşı and Yıldırım [78] employed ML techniques to examine the influence of material and deposition methods on the stability of PV cells. The findings of their research suggested certain materials with enhanced stability for PSCs, as detailed in the concluding section. Additionally, the study yielded other outcomes regarding methods and storage conditions that can contribute to increased stability and reduced degradation. These findings are presented in Table 5.

Table 5. Methods and storing conditions to reach higher stability and less degradation (based on the data from reference [78]).

Method and storing conditions	*Application*
multi-spin coating	one-step deposition
store in low humidity	Higher stability
store in dry condition [inverted cells]	Less degradation

4.1.3. Material properties prediction

In some papers, ML is used to predict material properties instead of direct material analysis. Consequently, with the knowledge of the properties of the suitable material, it could be easier to find materials with these properties. In 2019, Im et al. [79] used ML to try to find a way to find new lead-free perovskites. In this study, they tried to predict some material properties like the heat of formation (ΔHf) and bandgap (Eg) using the GBR Tree algorithm as accurate predictions, and electronically calculated data for compounds (A2B1+B3+X6) as training data. According to the results, the most important features in terms of ΔHf and Eg prediction were the space group of the crystal and the type of halogen anions, respectively.

Recognizing the relationship between the chemical structure and PV properties of materials is always a challenge. Predicting this relationship before materials are synthesized is a fundamental step forward in the search for high-performance materials for use in solar cells. To this end, in 2019, Sun et al. [80] developed a method for rapid material screening using a database of 1,719 types of (donor) and ML. In this study, five different algorithms were investigated for classifying and screening data. The proposed model was verified using 10 newly designed materials with A-π-D-π-A structure. In this structure, A is the end group, π is the link and D is the core. A, D, and π-D-π vary in each complex. According to the voltage-current diagram of these newly developed materials, the best material had an open circuit voltage (OCV) of 0.9 V and a Isc of 15.8 mA. The voltage and current range for all materials were between 0.8 V – 1.1 V and 4 Ma – 15.8 Ma, respectively. The Curie temperature or second-order temperature-phase transition is one of the most important factors of perovskite materials. In 2018, Zhai et al. [81] used ML to find new materials with higher Curie temperatures. Support Vector Machine (SVM), Relevance Vector Machine and RF algorithms to predict the Curie temperature of the materials. According to their results, [La0.66Sr0.3Ba0.04MnO3] has higher temperatures than the other data sets.

Realistic finite-temperature simulation of materials has always been a challenge for scientists and manufacturers and requires a lot of time and attention. In 2019, Jinnouchi et al. [82] attempted to automate this process using ML and used this model to find a relationship between the phase transition temperatures of different perovskites and the radii of the species involved. As a result, the proposed model was extended to estimate and compare the transition temperature of inorganic perovskites with ABX_3 structure.

In halide PSCs, the decomposition energy is closely related to the stability of the cells. In 2019, Zhenzho et al. [83] combined ML and DFT to propose a model containing the decomposition energies of 354 halide PSCs. The aim of this study was to find a relationship between decomposition energy and structural and chemical features. The stability prediction results for halide perovskites and mixed perovskites (with ABI3 and ApbX3) agreed well with the experimental results.

In 2019, Azri et al. [84] attempted to improve the efficiency of PSCs by using ML to propose high-performance materials for ETL and HTL layers. According to their results, zinc oxide (ZnO) and TiO_2 have the best potential for the ETL layer. Moreover, Copper(I) thiocyanate (CuSCN) is the best candidate for the HTL layer. As another result of this study, the thickness of the absorber

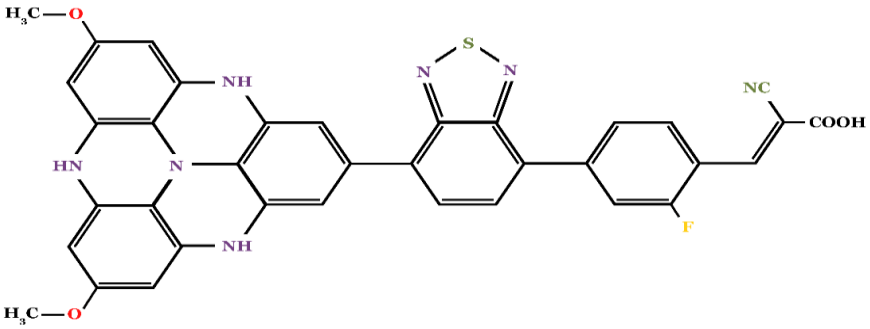
layer was optimized, and the optimal thickness was determined to be 1 µm. Considering all the results of this study, the cell has achieved more than 25% efficiency. In 2021, Yaoyao et al. [85] proposed a ML model to predict the band gap of various perovskite materials with CsaFAbMA [1-a-b] Pb [ClxBryI[1-x-y]] structure. In this formula, FA, and MA stand for formamidinium and methylammonium, respectively. The neural network had the best accuracy and according to the predicted results, the mixed halide perovskites had the best band gap and high iodide ratio. The results also show that the A-site cations (such as cesium, formamidinium, and methylammonium) have a strong influence on the band gap.

4.2. Application of ML in DSSCs

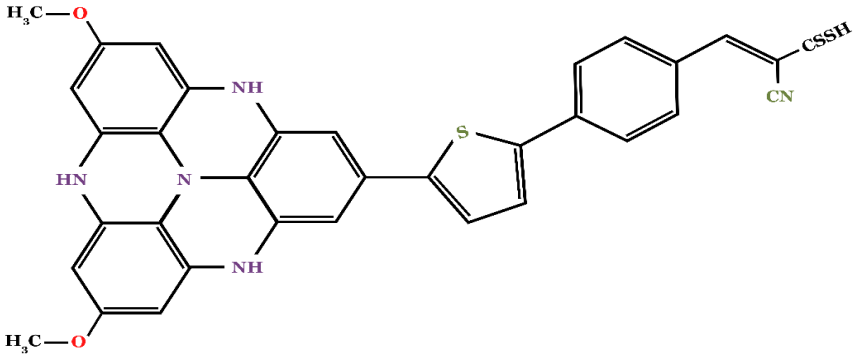
DSSCs have garnered attention due to the simplicity of their manufacturing process and their ongoing advancements. In this section, the articles published on the background of DSSCs and their association with ML tools are investigated. Based on recent research, ML has been primarily employed in DSSCs in four main areas: (1) Selection of appropriate materials for DSSCs, (2) Optimization of the fabrication process, (3) Prediction of material properties, and (4) Optimization of the device structure.

4.2.1. Selecting proper materials

In 2020, Wen et al. [86] utilized a combination of quantitative structure-property relationships and ML to identify novel dyes for DSSCs. They explored a database consisting of nearly 10,000 dyes and employed various ML algorithms, including RF, GBR Tree, SVM, and ANN, to mine the database. As a result, they identified eight potential organic dyes, all of which exhibited cell efficiencies exceeding 9%. Figure 5 presents the molecular structures of the two most efficient molecules. Molecule a demonstrated an efficiency of 10.2%, while molecule b exhibited an efficiency of 10.15%.



a.



b.

Figure 5. Structure of two new molecules with the highest efficiency [86].

In 2021, Wang et al. [87] used ML and chemical science to develop new donor-π-spacer acceptor dyes. The most important factor to determine the quality of new material for DSSCs is the ultraviolet–visible spectrum, which is calculated using the time-dependent DFT. The results of this study show that the mixture of 3,4-ethylene dioxythiophene, thiophene, and fluorene can improve the structure of π-spacers. It is also concluded that mixing π-units can be more effective than repeating them. One of the most important features to detect π-spacers is the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy gap. The frontier orbitals and their distributions are also important features for the development of new organic dyes.

4.2.2. Optimization of construction process

Dye enhancement plays a crucial role in determining the PV function of DSSCs. In 2020, Venkatraman [88] proposed a ML model based on molecular fingerprint-based methods to expedite the detection of aggregated J and H colors. A comprehensive database consisting of data from 3418 colors in 18 different solvents was meticulously compiled. These data were randomly partitioned into two categories: Test (20%) and Training (80%). Four algorithms, namely, classification and regression trees, RF, GBR trees, and SVM, were employed to classify the data. To evaluate the model's performance, the test pattern was subjected to a thousand random shifts to assess the accuracy for a thousand iterations. The results indicate that the random tree algorithm exhibited superior performance, achieving a higher accuracy of 75%. Table 4 presents the accuracy of the model stratified by solvent class. Notably, some combinations achieved a remarkable accuracy of 100%. The findings underscore the efficacy of the fingerprint method in swiftly and proficiently ascertaining the propensity of dyes towards J/H aggregation compared to alternative approaches.

4.2.3. Material properties prediction

In 2019, Arooj and Wang [89] attempted to improve DSSCs by determining the optical properties of dye molecules. The aim of this study was to find more efficient π-spacers for dyes with the donor-π-spacer-acceptor structure. Three π-spacer buildings, including 3,4-ethylenedioxythiophene (EDOT), fluorene, and thiophene, were considered as π-spacers for new dyes, and nine organic dyes were used to develop a ML model. According to their results, the repetition of fluorene in the structure of the π-spacer leads to an increase in the Ultraviolet (UV) spectral band of the donor. To increase the UV absorption, the use of fluorene and EDOT-π-spacer could be the key.

In 2020, Ju et al. [15] utilized GA and multiple linear regression to identify the crucial features of materials and utilized this data to develop novel N-annulated perylene sensitizers. A database consisting of 54 N-P dyes was compiled, aiming to develop dyes that could enhance the energy conversion efficiency by approximately 20%. Subsequently, energy conversion was calculated using density functional theory (DFT) and time-dependent density functional theory (TD-DFT), and the calculated values were compared with the predicted values obtained through GA. This study resulted in the design of five dye patterns, and the impact of these new dyes on solar cell performance was evaluated. For these newly developed dyes, the Isc ranged from 21.69 to 26.13 Ma.cm-2, the OCV ranged from 788 to 816 Mv, and the efficiency ranged from 12.99 to 15.16. A comparative analysis of these new dyes vis-à-vis the reference dyes revealed an increase in inefficiency ranging from 16.3 to 22.0%, a reduction in band gap of 11.1 to 20.6%, an increase in absorption wavelengths of 7.6 to 25.8%, and an increase in Isc of 10.6 to 20.5%.

In 2021, Santosh et al. [90] employed ML techniques (RF and ANN) to predict the efficiency of ZnO DSSCs under different synthesis conditions. The training dataset consisted of 70% of the collected database, while the remaining 30% was used as the test dataset. The model incorporated various input parameters, including structure, precursor, dye, seed layer, synthesis time, and temperature. The results demonstrated that the RF and ANN models achieved accuracies of 96.62% and 97.56%, respectively. The RF model predicted the highest efficiency of 6.2%, whereas the ANN model predicted it to be 5.8%. It is noteworthy that the Optimization of device Structure section provides detailed information on the optimal input parameters for achieving higher efficiency output.

Molecular functionalization can enhance the light-harvesting ability of porphyrins by modifying their physicochemical properties. In 2018, Li et al. [91] employed ML and chemical graph theory to predict the band gap of over 12,000 porphyrins. A training and validation dataset comprising 75% of the database was utilized, while the remaining 25% served as the test dataset. Several ML algorithms including Lasso, Kernel Ridge Regression, SVM, and Feedforward ANN were

employed to predict the band gap energy. From the results, it was observed that among the selected features, the pyrrole ring carbon associated with a single-bonded anchor group exhibited the highest importance. The results from DFT indicated that the LUMO state could facilitate the transfer of excited electrons to the oxide, thereby influencing the band gap in DSSCs.

In 2015, Li et al. [92] attempted to predict the efficiency of DSSCs using quantitative structure-activity relationship and ML. Thirty-one parameters were considered as input features, and Isc, OCV, fill factor (FF), and efficiency were defined as outputs. The main results of this study demonstrate that increasing the band gap energy leads to an increase in OCV. Furthermore, the efficiency of dye regeneration is significantly influenced by the HOMO energy. The predicted values for Isc, OCV, and efficiency ranged from 0.4 to 22.1 mAcm-2, 260 to 830 Mv, and 0.05 to 10.1%, respectively.

4.2.4. Device structure optimization

ZnO is a functional material extensively used in DSSCs. In 2020, Regonia et al. [93] employed several ML algorithms, including kernel ridge regression and ANN, to predict the band gap energy of ZnO and optimize the associated parameters. Zn2+ was utilized for the synthesis of ZnO quantum dots. The findings indicate that higher temperatures lead to increased quantum dot diameter and decreased band gap energy. Furthermore, it was observed that larger nanocrystals exhibit a smaller band gap.

TiO_2 is another widely used material for DSSCs. Surface area and lattice parameters are closely related to the TiO_2 band gap. In 2020, Zhang and Xu [94] attempted to predict the band gap of TiO_2 using Gaussian process regression based on surface area and lattice parameters. They investigated the band gap of 60 doped anatase TiO_2 photocatalysts and their model correlation with experimental results was almost 99.99%. According to their results, some complexes such as $S0.05Zn0.001/TiO_2$ and 1% Nb-doped TiO_2 had the highest band gap energy. They also concluded that some crystal defects could decrease the band gap and increase the efficiency of the photocatalyst. Moreover, the addition of some dopants such as N could increase the recombination of charge carriers and decrease the efficiency.

In 2021, Santosh et al. [90] employed decision trees, conventional decision trees, and classification and regression trees to investigate the relationship between cell efficiency and various ZnO synthesis parameters. The results demonstrated that synthesizing ZnO at temperatures above 100 ˚C and utilizing zinc nitrate precursors can enhance efficiency. Additionally, incorporating micro and 1D and 2D nanostructures under identical conditions showed potential for efficiency improvement.

4.3. Application of ML in SPR cells

As mentioned in previous sections, another nano-based solar cell is the SPR cell, which leverages the phenomenon of SPR with conduction layer electrons [53]. SPR cells have received relatively less attention in previous review articles. Therefore, this section aims to discuss the applications of ML in the advancement of SPR solar cells from various perspectives. Based on the classification employed in this study, the applications of ML in SPR solar cells can be categorized into two primary groups: device structure optimization and material property prediction.

4.3.1. Device structure optimization

One of the practical solutions to improve the performance of solar cells is to improve light absorption, which directly affects the efficiency and production capacity. In 2008, Lin and Phillips [25] used a GA to optimize multilevel rectangular and arbitrary networks in thin-film cells with a ZnO/a-Si/ZnO/Ag structure. Their goal was to capture light and improve the utilization of sunlight. To this end, the performance of different cell types was studied including solar cells with optimized multilevel rectangular gratings, flat cells, optimal cells with periodic gratings, and solar cells with optimized gratings. The conversion efficiencies for these cells were calculated using Maxwell's equations. According to the results of this study, the optimized multilevel rectangular lattices produced a 23% improvement in flat cells and a 3.8% improvement for the best cells with a periodic lattice. According to the authors of the study, this improved behavior was the result of the pairing of light and the effects of capturing a broad spectrum of sunlight. Optimized custom grids further enhanced this effect. There was a 29% improvement in flat cells and a 9% improvement with the best periodic reticulum.

In 2010, Forestiere et al. [26] employed the PSO algorithm to design metal nanoparticle arrays that enhance the bandwidth of the plasmonic field in the visible light spectrum. The results indicated that the maximum enhancement occurs at a

wavelength of 500 nm. It was ultimately concluded that the increase in nanoplasmonic field bandwidth can be achieved through the design of periodic arrays with a multitude of spatial frequencies, facilitating the necessary interaction between diffraction phenomena at multiple scales and quasi-static binding in small nanoparticles.

In 2015, Rahmani et al. [27] used PSO to optimize the structure and thickness of organic nano-based solar cells of methyl ester poly [3-hexylthiophene] and [6,6] phenyl C61-butyric acid. A function with three variables was considered, including the size, amplitude, and thickness of the active layer. According to the results, the optimal size was 17 nm. It was also found that the maximum Isc was about 11mAcm-2, which is the case when the circumference of the active layer girth of 200 nm.

In 2015, Aiello et al. [95] optimized the size and position of metal nanoparticles in plasmonic cells through the utilization of GA and metaheuristic algorithms. The primary objective of this research was to decrease the thickness of the cells without compromising their efficiency by incorporating silver nanoparticles, while simultaneously reducing the usage of silver. An objective function was defined as follows [95]:

$$F[d,h,r]=\frac{1}{\lambda_E-\lambda_S}\int_{\lambda_S}^{\lambda_E}\eta_\lambda(d,h,r)d\lambda \qquad (1)$$

In equation 1, η_λ is the function of the geometric parameters. Λ and F are the wavelength and the objective function, respectively. According to the first optimal solution, 60% silver was saved (98 mg/m^2 instead of 241 mg/m^2), while the objective function decreased by only 1%. In the second solution, the amount of silver used was drastically reduced (38 mg/m2), but the value of the objective function was about 5% worse.

4.3.2. Material properties prediction

In 2020, Che Yen et al. [96] used ML to find the relationship between material properties and synthesis. In this context, a limited database was collected, and ANN and GA were used to develop the model. The results show that the efficiency of SPR effects of Au/ZnO can be evaluated by ML. Moreover, the model ANN/GA was very accurate, and the main predicted results of the model were the position of the absorption peak, the efficiency, and the Q factor.

5. Conclusion

In this study, we investigated the development of three types of PSCs, DSSCs, and SPR solar cells using ML approaches and algorithms. We presented articles on these topics to contribute to the existing knowledge.

PSCs have gained popularity in both the field of solar cells and among researchers in recent years due to their rapid development and high efficiency. According to the research conducted in this article, most of the articles published on the three types of cells discussed in relation to ML had a significant focus on PSCs. The majority of the published articles in the field of PSCs and ML were related to the discovery of new materials with improved performance and the prediction of material properties. Moreover, ML techniques were applied to address the stability and structural optimization of PSCs. The stability of PSCs is an important challenge, and ML can serve as a low-cost and efficient tool to enhance their stability. Based on our classification in this study, the applications of ML in PSCs can be categorized into three main groups: material selection, design optimization, and material property prediction.

As for DSSCs, despite their lower efficiency, they are relatively easier to manufacture and have gained popularity. The number of published articles on DSSCs and ML was comparably lower than that of PSCs. The primary application of ML to this type of cell involved discovering new color compounds with higher efficiency. Structural optimization and performance prediction of DSSCs were also addressed using data mining and ML techniques. Considering that DSSCs are still in the early stages of development, ML can prove to be a powerful tool for advancing these cells and expediting their progress. In this study, ML applications in DSSCs were categorized into four main areas: material selection, design optimization, material property prediction, and device structure optimization.

Lastly, we discussed SPR cells in this article. The number of published ML articles on SPR cells was considerably lower compared to other types of solar cells. ML and its algorithms primarily contributed to optimizing the structure and improving the performance of SPR cells. Notably, maximizing light absorption in these cells was identified as a crucial technique for optimizing their structure. The applications of ML in SPR cells can be divided into two groups: device structure optimization and material property prediction.

Overall, this study provides valuable insights into the applications of ML in various types of solar cells, highlighting their potential for material discovery, design optimization, and performance prediction. The results obtained pave the way for

future advancements and improvements in the field of solar cell technology.

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کاربرد الگوریتم های یادگیری ماشین در بهبود فناوری سلول های خورشیدی مبتنی بر نانو

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چکیده:

این مطالعه به بررسی پتانسیل استفاده از تکنیک‌های یادگیری ماشین برای تقویت سه نوع سلول خورشیدی مبتنی بر نانو می‌پردازد. پروسکایت‌های فرمیدینیم بدون متیل آمونیوم و سلول‌های مبتنی بر کاتیون‌های مخلوط، کارایی افزایش یافته‌ای را هنگام استفاده از تکنیک‌های یادگیری ماشین نشان می‌دهند. علاوه بر این، روش‌های یادگیری ماشین برای شناسایی ترکیب‌های اهداکننده بهینه، مواد با دمای کور بالا و پیشبرد پایداری ترمودینامیکی پروسکایت‌ها مورد استفاده قرار می‌گیرند. یکی دیگر از کاربردهای مهم یادگیری ماشین در سلول‌های خورشیدی حساس به رنگ شناسایی رنگها، حلال‌ها و مولکولهای جدید برای بهبود کارایی و عملکرد سلول‌های خورشیدی است. برخی از این مواد بازده سلول، جریان اتصال کوتاه و جذب نور را بیش از ۲۰ درصد افزایش داده‌اند. الگوریتم‌های یادگیری ماشین برای تنظیم دقیق پهنای باند شبکه و میدان پلاسمونیک، کارایی و جذب نور سلول‌های خورشیدی رزونانس پلاسمونیک سطحی را بهبود می‌بخشند. این مطالعه پتانسیل تکنیک‌های یادگیری ماشین را برای بهینه‌سازی و بهبود توسعه سلول‌های خورشیدی مبتنی بر نانو نشان می‌دهد که منجر به نتایج امیدوارکننده‌ای برای زمینه تولید انرژی خورشیدی و حمایت از تقاضا برای انرژی پایدار و قابل اعتماد می‌شود.

کلمات کلیدی: یادگیری ماشین، بهینه‌سازی، سلول خورشیدی، سلول خورشیدی نانوساختار.