

SPECIAL ISSUE Thematic Collection: Powering the Future:
Advancements in Clean, Affordable, and Renewable Energy for
Sustainable Development

REVIEW ARTICLE **OPEN ACCESS**

Accelerating Organic Solar Cell Development Through Artificial Intelligence–Driven Material Discovery and Optimization

Marwan Al-Raei^{1,2,3} 

¹Damascus University, Damascus, Syria | ²Al-Andalus University for Medical Sciences, Tartus, Syria | ³International University for Science and Technology, Ghabagheb, Syria

Correspondence: Marwan Al-Raei (mn41@live.com; mhdm-ra@scs-net.org)

Received: 25 April 2026 | **Revised:** 31 July 2026 | **Accepted:** 4 August 2026

Guest Editor: Claire Gao

Keywords: artificial intelligence | device optimization | machine learning | material discovery | organic solar cells

ABSTRACT

The development of organic solar cells (OSCs) holds great promise for sustainable energy due to their lightweight, flexibility, and potential for low-cost production. However, challenges such as material discovery, device optimization, stability, and morphological control hinder their commercial viability. Recent advances in artificial intelligence (AI) and machine learning (ML) offer transformative solutions to accelerate progress across these domains. In this article, we focus on how AI techniques facilitate high-throughput virtual screening of organic materials, optimize fabrication parameters through Bayesian methods, predict long-term stability, and analyze nanoscale morphology via automated image recognition. By leveraging large datasets and predictive models, researchers can efficiently narrow down the vast chemical space to identify promising donor and acceptor molecules with desirable electronic properties, such as optimized highest occupied molecular orbital (HOMO)/lowest unoccupied molecular orbital (LUMO) levels. AI-driven virtual screening significantly reduces experimental costs and time, guiding synthesis toward high-potential candidates. Additionally, AI algorithms like Bayesian optimization (BO) streamline the tuning of fabrication processes, solvent selection, coating speed, and annealing conditions, leading to improved active layer morphology and device performance with fewer trials. Predictive models based on recurrent neural networks (RNNs) and long short-term memories (LSTMs) enable the forecasting of degradation mechanisms, informing the design of more durable materials and encapsulation strategies. Automated convolutional neural networks (CNNs) facilitate detailed morphological analysis, establishing correlations between nanoscale phase separation and efficiency. Furthermore, explainable AI (XAI) approaches enhance transparency, enabling researchers to interpret model decisions, identify key features influencing performance, and make targeted improvements. Looking ahead, emerging AI paradigms such as generative models, autonomous laboratories, and digital twins promise to revolutionize OSC research, accelerating the discovery of high-efficiency, stable, and environmentally sustainable organic photovoltaic devices. The integration of AI thus represents a pivotal step toward realizing the full potential of OSCs in renewable energy applications.

This is an open access article under the terms of the [Creative Commons Attribution](https://creativecommons.org/licenses/by/4.0/) License, which permits use, distribution and reproduction in any medium, provided the original work is properly cited.

Copyright © 2026 Marwan Al-Raei. *International Journal of Energy Research* published by John Wiley & Sons Ltd.

1 | Introduction

The quest for sustainable and effective energy solutions has emerged as one of the most pressing scientific and technological issues of the 21st century [1, 2]. Within the spectrum of renewable energy technologies, solar power is particularly notable for its vast availability and eco-friendliness [3]. Specifically, photovoltaic systems have undergone remarkable progress in recent decades, fueled by breakthroughs in materials and device configurations [4, 5]. While conventional silicon-based solar cells have reached impressive efficiency levels, their production costs and constraints regarding flexibility and lightweight applications have prompted the investigation of alternative materials and innovative designs [1, 6]. Organic solar cells (OSCs) have emerged as a promising renewable energy technology due to their potential for lightweight, flexible, and cost-effective photovoltaic devices [7]. Over the past decades, significant efforts have been directed toward enhancing their power conversion efficiency (PCE), stability, and manufacturability [8]. Despite these advancements, the development of high-performance OSCs remains a complex challenge, primarily due to the vast and intricate chemical space of organic materials and the multifaceted nature of device fabrication and operation [7, 9, 10]. Traditionally, the discovery and optimization of suitable donor and acceptor materials, as well as device fabrication parameters, relied heavily on experimental trial-and-error approaches. These methods, while valuable, are inherently time-consuming, resource-intensive, and limited in their capacity to explore the enormous diversity of potential materials and processing conditions [11, 12].

The core challenge in improving OSC performance lies in identifying optimal combinations of organic materials that can efficiently absorb sunlight, facilitate effective charge separation, and enable charge transport with minimal recombination. The efficiency of an OSC is critically dependent on the electronic properties of the constituent materials, particularly their energy levels, such as the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) [13, 14]. Precise tuning of these energy levels is essential to maximize open-circuit voltage (V_{oc}) and short-circuit current density (J_{sc}), which collectively influence overall efficiency. However, the sheer number of possible molecular structures and their combinations makes manual screening impractical [15, 16].

In recent years, the advent of artificial intelligence (AI) and machine learning (ML) techniques has revolutionized the landscape of material discovery and device optimization. These computational approaches, as illustrated in Figure 1, offer powerful tools to navigate the expansive chemical space efficiently, predict key electronic and morphological properties, and guide experimental efforts toward the most promising candidates [17, 19, 20]. By leveraging large datasets and sophisticated algorithms, researchers can perform high-throughput virtual screening to rapidly identify potential donor and acceptor molecules with desirable energy levels and absorption characteristics [21, 22]. This virtual screening paradigm allows for the rapid narrowing down of candidate materials, significantly reducing the time and cost associated with traditional experimental screening [17, 19].

AI-driven methods excel in modeling complex relationships between molecular structures and their electronic properties. Molecular representations such as graphs and simplified molecular-input line-entry system (SMILES) strings serve as input features for training predictive models. Once trained on existing datasets, these models can accurately forecast properties like HOMO/LUMO energies, maximum absorption wavelength (λ_{max}), and charge carrier mobility (μ) for novel molecules, enabling researchers to prioritize candidates for synthesis and testing [22–24]. Furthermore, AI can incorporate predictive models based on physical principles, such as the Scherbar model, to estimate the potential efficiency of OSCs based on material energy levels, thus refining the screening process.

Beyond material selection, AI techniques extend to optimize device fabrication parameters, which are equally critical for achieving high performance [25–27]. The active layer morphology, which is the layer of an OSC typically consists of a blend of donor and acceptor materials, influenced by variables such as solvent choice, coating speed, and annealing conditions, plays a pivotal role in charge transport and recombination dynamics. Traditional optimization methods often involve extensive experimental iterations; however, AI-based algorithms like Bayesian optimization (BO) facilitate systematic and efficient exploration of multidimensional parameter spaces. BO employs probabilistic models, such as Gaussian processes (GPs), to predict performance outcomes and iteratively suggest the most promising parameter combinations based on previous experimental data. This approach accelerates the identification of optimal fabrication recipes, leading to improved device morphology and enhanced efficiency with fewer trials [9, 19, 28]. Furthermore, AI techniques contribute to the understanding and prediction of long-term stability and degradation mechanisms, which are vital for commercial viability. By analyzing accelerated aging data through ML models like recurrent neural networks (RNNs) and long short-term memory (LSTM) networks, researchers can forecast device lifetime and identify structural features associated with degradation pathways. Such insights guide the design of more stable organic materials and encapsulation strategies, ultimately extending the operational lifetime of OSCs.

In this article, we focus on the transformative role of AI techniques in the high-throughput virtual screening of materials for OSCs. We explore how AI accelerates the discovery of promising donor and acceptor molecules, optimizes fabrication parameters through Bayesian methods, predicts device stability, and analyzes morphological features via advanced image recognition. By examining these interconnected aspects, we aim to highlight the significant advancements AI has brought to the field of OSC research, paving the way toward more efficient, stable, and commercially viable organic photovoltaic devices.

2 | AI for Materials of OSCs

In this section, we focus on how AI techniques explore high-throughput virtual screening of materials in OSCs. A significant hurdle in the development of OSCs is the identification of optimal donor and acceptor material combinations. The efficiency of

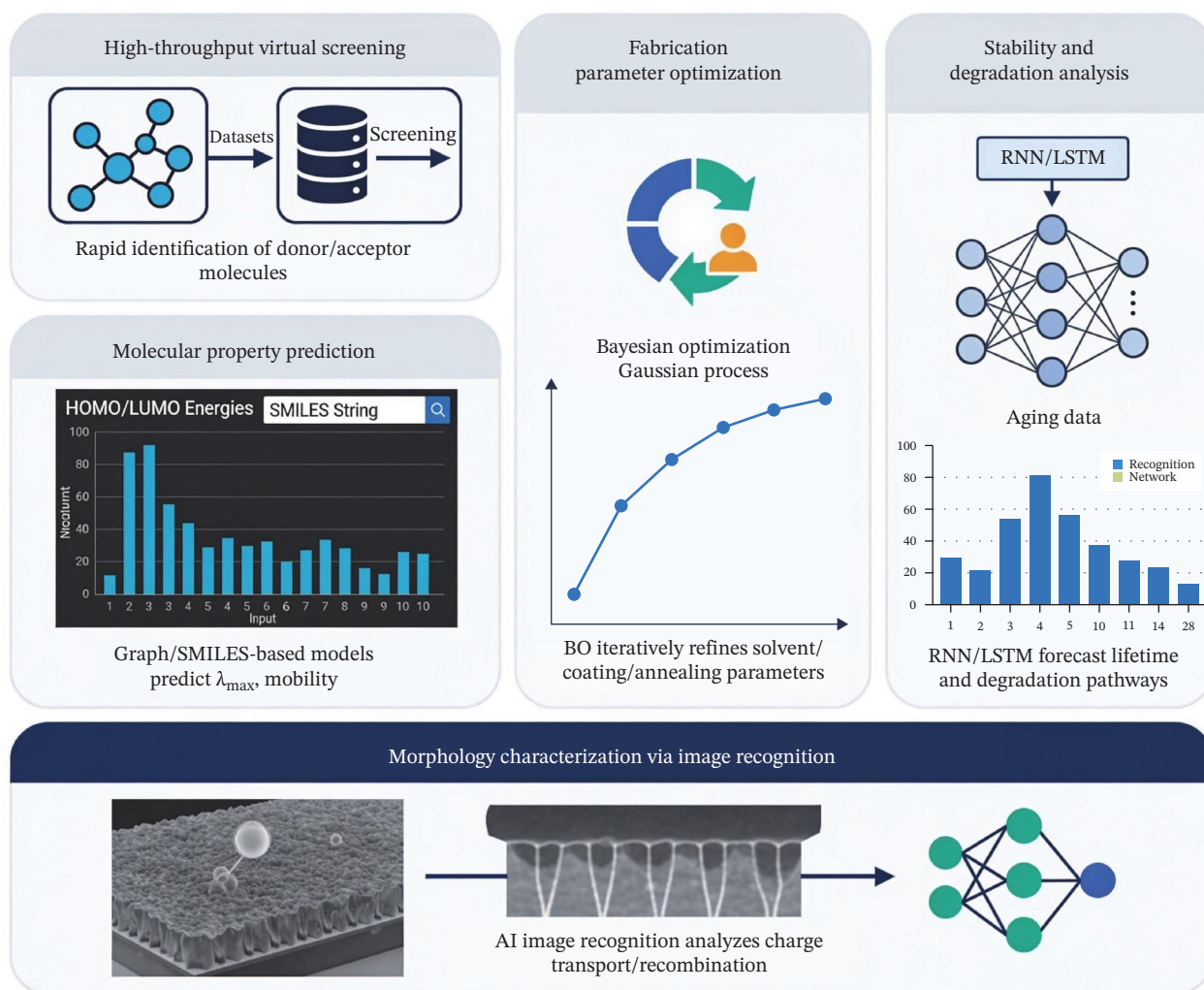


FIGURE 1 | Possible advancement of AI in organic solar cell developments [17, 18].

these solar cells is critically influenced by the electronic properties of the materials, particularly their capacity to absorb light and facilitate charge separation and transport.

2.1 | The Challenge of Material Selection

The extensive chemical space available for organic materials presents a formidable challenge for researchers. With millions of potential organic molecules, the traditional method of synthesizing and testing each candidate in the laboratory is not only time-consuming but also resource-intensive. The PCE of an OSC is defined as [29]:

$$\text{PCE} = \frac{J_{\text{sc}} \cdot V_{\text{oc}} \cdot \text{FF}}{P_{\text{in}}}, \quad (1)$$

where:

- J_{sc} is the short-circuit current density expressed in A/m^2 ,
- V_{oc} is the open-circuit voltage expressed in volts,
- FF is the fill factor, which is unitless factor, and

- P_{in} is the incident solar power expressed in watt.

The challenge lies in maximizing J_{sc} and V_{oc} , which are directly influenced by the energy levels of the donor and acceptor materials. The open-circuit voltage, applied for OSCs [30, 31], can be approximated by the difference between the HOMO level of the donor $E_{\text{HOMO}}^{\text{Donor}}$ and the LUMO level of the acceptor $E_{\text{LUMO}}^{\text{Acceptor}}$ [30]:

$$V_{\text{oc}} \approx \frac{1}{e} \left(|E_{\text{HOMO}}^{\text{Donor}}| - |E_{\text{LUMO}}^{\text{Acceptor}}| \right) - \Delta V, \quad (2)$$

where ΔV accounts for empirical losses expressed in volts, the energy levels are expressed in joule, and e is the charge of the electron, which is expressed in coulomb. This equation underscores the necessity of selecting materials with appropriate energy levels to achieve high efficiency. The approximation of open-circuit voltage assumes that the energy levels of the donor and acceptor materials are well-aligned to facilitate efficient charge transfer, which is crucial for optimizing the performance of OSCs. Additionally, it presumes that the system operates under ideal conditions, where factors such as temperature and

light intensity are controlled. Equation (2) highlights the importance of selecting donor and acceptor materials with suitable energy levels to maximize the open-circuit voltage and, consequently, the overall efficiency of the solar cell.

2.2 | How AI Facilitates Virtual Screening

AI and ML have emerged as transformative tools to tackle this challenge. Instead of relying solely on physical synthesis, researchers can utilize ML algorithms to conduct virtual screenings of extensive databases containing millions of potential organic molecules. This approach significantly accelerates the identification of promising candidates.

AI models can be trained to predict essential electronic properties such as HOMO and LUMO energy levels based on molecular structures. In Table 1, we summarize the key electronic properties of organic materials that are critical for the performance of OSCs. Understanding these properties is essential for optimizing material selection and enhancing solar cell efficiency. This is accomplished by representing molecules as graphs or using SMILES strings. The mapping function *f* can be expressed as [18]:

f(“Molecular Structure”) → {E_{HOMO}, E_{LUMO}, λ_{max}, μ}, (3)

where λ_{max} is the wavelength of maximum absorption expressed in meters, and μ is the charge carrier mobility expressed in m²/(sVolts). By training these models on existing datasets, researchers can predict the properties of new molecules with high accuracy and speed.

2.3 | Impact of AI on Material Selection

The impact of AI in this context is profound. By employing ML models, researchers can narrow down the search space from millions of candidates to select a few high-potential molecules that merit further experimental investigation. This not only conserves time but also optimizes resource allocation, allowing researchers to concentrate on the most promising candidates for synthesis and testing.

AI-driven approaches can also incorporate various predictive models, such as random forests or neural networks, to evaluate the likelihood of achieving high PCE based on the selected materials. The Scharber model [32], which correlates OSC efficiency with material energy levels, can be utilized to effectively filter candidates [32, 33]:

TABLE 1 | Key electronic properties of organic materials for organic solar cells (OSCs).

Property	Symbol	Relevance to OSC performance
HOMO	E _{HOMO}	Determines open-circuit voltage (V _{oc}) and influences charge separation efficiency
LUMO	E _{LUMO}	Affects V _{oc} and the energy barrier for electron transfer
Maximum absorption wavelength	λ _{max}	Critical for optimizing light harvesting and overall energy conversion efficiency
Charge carrier mobility	μ	Essential for efficient charge transport and minimizing recombination losses

η = (FF · V_{oc} · ∫_{E_g}[∞] Φ_{ph}(E)dE) / P_{total}, (4)

where η is the efficiency, FF is the fill factor, Φ_{ph}(E) is the photon flux, and the denominator represents the total incident power of the cell. This model enables researchers to prioritize candidates that are likely to achieve efficiencies above a specified threshold.

The main advantages can be shown by comparison between experimental results of OSC materials and AI approaches. Table 2 contrasts the advantages and limitations of experimental results versus AI-predicted outcomes. While experimental methods provide direct measurements, they are often limited by time and resources. In contrast, AI predictions allow for rapid exploration of chemical spaces but may overlook certain complexities inherent in real-world materials. Besides, there are other approaches included as follows:

- Hybrid approach: This methodology combines the strengths of both experimental and AI predictions. While it can lead to high accuracy, it requires careful integration and validation, which can complicate the process and extend the timeframe.
- Theoretical calculations: These calculations offer insights into the fundamental properties of materials based on theoretical models. Although they can be cost-effective, they may rely on simplifying assumptions that do not fully capture the complexities of real-world materials, leading to variable accuracy.
- Expert evaluation: This approach utilizes the experience and intuition of researchers in the field. While it can yield high accuracy, it is subjective and may introduce bias, making it less reliable in some cases.

By comparing these methodologies, researchers can better understand the strengths and weaknesses of each approach, allowing for more informed decisions in the material selection process for OSCs. Ultimately, a combination of methods may provide the most robust pathway to discovering and optimizing new materials for OSC applications. As a result of that, while AI models significantly enhance the efficiency of material selection for OSCs, it is crucial to acknowledge their limitations. The predictions made by AI may not always align with experimental results due to factors such as unaccounted interactions, material imperfections, or environmental conditions. Therefore, a balanced approach that combines AI predictions with experimental validation is essential for advancing the field of OSCs.

TABLE 2 | Comparison of methodologies for material selection in organic solar cells.

Methodology	Advantages	Limitations	Typical timeframe	Cost implications	Accuracy level
Experimental results	Direct measurement of material properties	Time-consuming and resource-intensive	Weeks to months	High (materials and labor costs)	High (if well-controlled)
AI-predicted outcomes	Rapid screening of extensive chemical spaces	May overlook complex interactions	Days to weeks	Low (computational resources)	Variable (depends on model)
Hybrid approach	Leverages strengths of both experimental and AI methods	Requires careful integration and validation	Variable (scope-dependent)	Moderate (combined costs)	High (if properly validated)
Theoretical calculations	Insight into fundamental properties	Relies on simplifying assumptions	Variable (complexity-dependent)	Low to moderate (software tools)	Variable (model fidelity)
Expert evaluation	Utilizes domain expertise	Subjective, potential for bias	Variable	Moderate (consultation fees)	High (if expert is informed)

3 | Optimization of OSCs

In this section, we examine the optimization of device fabrication, focusing on the “Recipe” problem. Even when optimal materials are identified, the performance of an OSC is significantly affected by the fabrication process. The “recipe” for creating the active layer encompasses numerous variables, including solvent selection, material concentration, spin-coating speed, and annealing temperature. Each of these factors can profoundly influence the morphology of the active layer and, consequently, the efficiency of the solar cell.

3.1 | The Complexity of Fabrication Parameters

The active layer of an OSC typically consists of a blend of donor and acceptor materials, and its morphology is vital for achieving high performance [34]. The performance P_c can be expressed as a function of multiple parameters [35, 36]:

$$P_c = f(c, s, \omega, r, T_a, t_a), \tag{5}$$

where:

- c is the concentration of the active materials,
- s is the solvent type,
- ω is the spin-coating speed,
- r is the film thickness,
- T_a is the annealing temperature, and
- t_a is the annealing time.

Table 3 outlines the key fabrication parameters that influence the performance of OSCs. Each parameter is described along with its impact on the performance, emphasizing the importance of optimizing these variables to achieve high efficiency. The interaction between these parameters can lead to significantly different morphologies and efficiencies.

TABLE 3 | Key fabrication parameters influencing organic solar cell (OSC) performance.

Parameter	Symbol	Impact on performance
Concentration	c	Optimizes charge transport and affects blend morphology
Solvent type	s	Determines film formation and influences morphology
Spin-coating speed	ω	Affects film thickness and uniformity, impacting charge extraction
Film thickness	r	Influences light absorption and charge transport efficiency
Annealing temperature	T_a	Enhances crystallinity, affecting charge mobility and morphology
Annealing time	t_a	Impacts stability and morphology, influencing overall device performance

Optimizing these parameters is crucial for achieving the desired morphology that maximizes charge transport and minimizes recombination losses.

3.2 | How AI Assists With Optimization

To address the complexity of optimizing these fabrication parameters, researchers utilize BO, a powerful AI technique adept at optimizing multivariable processes. BO employs a probabilistic model to predict the performance of various parameter combinations and iteratively refines its predictions based on experimental outcomes. The Bayesian model employs a GP as a surrogate for the objective function, enabling researchers to estimate the mean $\mu(x)$ and variance $\sigma^2(x)$ of the performance [37, 38]:

$$P_c(x) \sim \text{GP}(\mu(x), k(x, x')), \tag{6}$$

where $k(x, x')$ is the covariance function. The GP provides a flexible framework for modeling the underlying function that connects fabrication parameters to performance.

3.3 | Acquisition Function for Sampling

To determine the next set of parameters to test, the AI utilizes an acquisition function, such as Expected Improvement (EI), which quantifies the potential benefit of sampling a new point [39–41]:

$$EI(x) = E[\max(f(x) - f(x^+), 0)], \tag{7}$$

where $f(x^+)$ represents the best observed performance to date. This approach allows the AI to balance exploration (testing new areas of parameter space) and exploitation (refining good known areas).

3.4 | Impact on Efficiency and Morphology

The implementation of AI-driven BO has a significant impact on the optimization of OSC fabrication. By systematically exploring the parameter space, researchers can identify the optimal “recipe” that results in the best morphology and performance, requiring significantly fewer experimental trials compared to traditional methods.

For instance, AI can recommend specific combinations of solvent types and spin-coating speeds that lead to optimal domain sizes, thereby enhancing charge transport and minimizing recombination. This optimization process not only accelerates the development of high-efficiency OSCs but also reduces the overall costs and time associated with the fabrication process. Consequently, the integration of AI in the optimization of device fabrication for OSCs addresses the intricate interplay of variables that influence performance. By leveraging BO, researchers can efficiently navigate the parameter space, leading to the development of high-performance OSCs. Table 4 compares traditional optimization methods with AI-driven approaches. While traditional methods provide direct experimental results, they are often time-consuming and resource-intensive. In contrast, AI-driven optimization allows for rapid exploration of the parameter space, leading to significant efficiency improvements. However, it requires initial data for effective model training, and integrating AI with traditional methods can introduce complexity.

By understanding the implications of these AI techniques, researchers can better navigate the optimization process for

OSC fabrication, leveraging both traditional and AI-driven approaches to enhance the performance of OSCs.

4 | AI and Stability of Solar Cells

In this section, we explore the prediction of long-term stability and degradation in OSCs. A significant challenge hindering the commercialization of OSCs is their long-term stability. Organic materials are inherently vulnerable to environmental factors such as oxygen, moisture, and heat, which can lead to degradation over time. We will examine how AI can be utilized to predict the long-term stability and degradation mechanisms of OSCs.

4.1 | Understanding Degradation Mechanisms

The degradation of OSCs is typically characterized by a multi-phase process, which includes an initial “burn-in” phase, followed by a steady-state degradation phase. Table 5 outlines the key factors that influence the degradation of OSCs. Each factor is described along with its impact on the stability of the solar cells. Understanding these factors is crucial for developing strategies to enhance the longevity of OSCs. The normalized PCE over time t can be modeled as follows [35, 42]:

$$\eta_n(t) = A_{bi}\exp(-k_{bi}t) + (1 - A_{bi})\exp(-k_s t), \tag{8}$$

where:

- A_{bi} is the amplitude of the burn-in phase,
- k_{bi} is the rate constant for the burn-in phase, and

TABLE 5 | Key factors influencing degradation in organic solar cells (OSCs).

Factor	Impact on stability
Oxygen exposure	Leads to oxidation of organic materials, compromising performance
Moisture content	Affects the integrity of the active layer, potentially causing delamination
Temperature	Influences reaction rates and material stability, affecting longevity
Light intensity	Accelerates photodegradation processes, reducing efficiency over time
Chemical structure	Determines susceptibility to degradation, influencing overall stability

TABLE 4 | Comparison of optimization approaches for organic solar cell (OSC) fabrication.

Approach	Advantages	Limitations	Efficiency improvement potential
Traditional optimization	Provides direct experimental results	Time-consuming and resource-intensive	Low to moderate
AI-driven optimization	Enables rapid exploration of parameter space	Requires initial data for model training	High
Hybrid approach	Leverages strengths of both traditional and AI methods	Complexity in integration and validation	Moderate to high

- k_s is the steady-state degradation rate.

The challenge lies in accurately predicting the values of k_{bi} and k_s based on the chemical structure of the materials and the environmental conditions they are exposed to.

4.2 | How AI Analyzes Accelerated Aging Data

AI models, particularly RNNs and LSTM networks, are effective in analyzing accelerated aging data to forecast how OSCs will perform over extended periods. These models consider various factors such as temperature T , humidity RH, and light intensity I to estimate the degradation rate k via defined by statistical distributions functions as [43, 44]:

$$k = A \cdot I^\alpha \cdot \exp\left(\frac{-E_a}{k_B T}\right) \cdot f(RH), \quad (9)$$

where:

- E_a is the activation energy for degradation,
- k_B is the Boltzmann constant, and
- $f(RH)$ is a function that describes the effect of humidity on degradation.

By training on historical data from accelerated aging experiments, AI can uncover patterns and correlations that may not be evident through traditional analytical methods.

4.3 | Impact on Material Design

The ability to predict degradation rates has profound implications for designing more durable organic materials. By identifying structural features that correlate with high degradation rates, researchers can modify chemical structures to enhance stability. For instance, AI can assist in designing molecules that are less prone to oxidation or that exhibit improved thermal stability.

Furthermore, AI can optimize encapsulation strategies by simulating interactions between the organic layer and barrier materials. AI-driven simulations can guide the selection of encapsulation materials and designs that minimize moisture ingress, thereby prolonging the operational lifetime of OSCs.

As a result of that, the integration of AI in predicting long-term stability and degradation mechanisms in OSCs represents a significant advancement in the field. By leveraging ML models to analyze accelerated aging data, researchers can design more robust organic materials and optimize encapsulation strategies, ultimately enhancing the commercial viability of OSCs.

On the other hand, there are limitations of accelerated aging datasets in the field of OSCs. Table 6 highlights the limitations of accelerated aging datasets when predicting the real operational lifetimes of OSCs.

The discrepancies between laboratory conditions and real-world environments can lead to inaccurate predictions of performance. Additionally, the short duration of accelerated aging tests may

TABLE 6 | Limitations of accelerated aging datasets in predicting real operational lifetimes of organic solar cells (OSCs).

Limitation	Impact on predictions
Environmental variability	Laboratory conditions may not replicate real-world environments, leading to inaccurate performance forecasts
Short testing duration	Limited duration of tests fails to capture long-term degradation trends, compromising reliability
Simplified conditions	Exclusion of critical environmental factors (e.g., pollution) can result in overly optimistic lifetime estimates
Material variability	Variations in material batches can affect results, reducing reproducibility and data reliability
Lack of real-time data	Insufficient access to real-time operational data limits the accuracy of predictions regarding long-term performance

not capture long-term degradation trends, and simplified testing conditions can overlook critical environmental factors that affect stability. Material variability and the lack of real-time operational data further complicate the ability to make reliable predictions.

By recognizing these limitations, researchers can better interpret the results of accelerated aging studies and develop more effective strategies for improving the stability and longevity of OSCs in real-world applications.

5 | Image Analysis of OSCs

In this section, we demonstrate the use of automated image analysis of morphology through convolutional neural networks (CNNs), as illustrated in Figure 2. The efficiency of an OSC is closely related to its morphology, which refers to the microscopic arrangement of donor and acceptor materials at the nanoscale. Understanding and quantifying this morphology are essential for optimizing device performance. We will explore how AI, specifically CNNs, can be utilized for automated image analysis of OSC morphology.

5.1 | The Importance of Morphology in OSC Performance

The morphology of the active layer in an OSC determines the pathways for charge transport and the efficiency of exciton dissociation. The relationship between morphology and performance can be complex, as the size and distribution of domains affect charge carrier mobility and recombination rates, which are related to the definition of the current density J [47, 48].

If morphology is poorly optimized, the mobility μ can drop significantly, leading to reduced current density and overall efficiency.

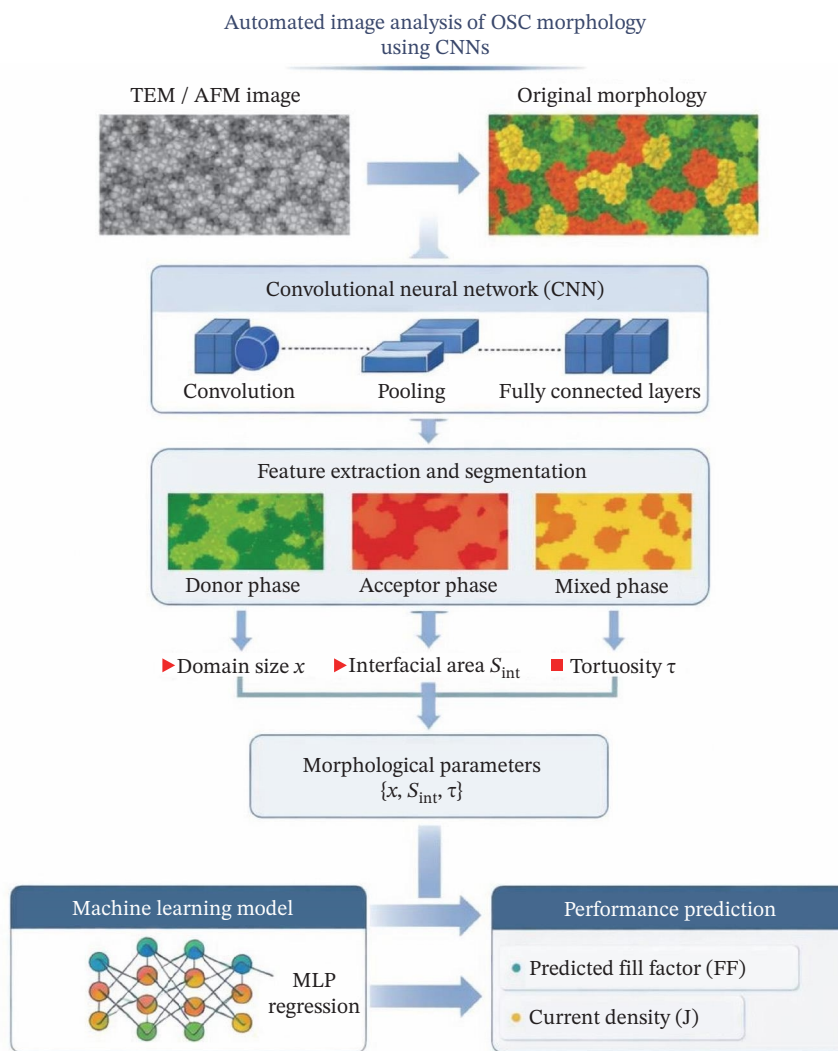


FIGURE 2 | Understanding OSC morphology and predicting performance use of AI image analysis of the variables and parameters [45, 46].

5.2 | How AI Facilitates Image Analysis

Historically, the analysis of images obtained from electron microscopes (TEM/SEM) or atomic force microscopy (AFM) has relied heavily on manual and subjective interpretation. However, the introduction of AI has enabled researchers to employ CNNs for automated image analysis. CNNs are particularly effective for image recognition tasks due to their capacity to learn hierarchical features directly from raw pixel data.

The architecture of a CNN comprises several layers, including convolutional layers, pooling layers, and fully connected layers [49, 50]. The convolution operation [51, 52] is fundamental to the functioning of CNNs [45, 46]. In addition, CNN methods are applied for discrete 2D images with its convolution operation [53, 54]. This convolution operation enables the CNN to extract critical features from the images, such as domain size, crystallinity, and phase separation. By automating this analysis, AI significantly enhances the efficiency and accuracy of image interpretation, allowing researchers to focus on more complex

analyses and interpretations of the morphological characteristics of materials.

5.3 | Impact: From Image Features to Performance Prediction

AI can quantify complex patterns in microscopy images that are often invisible or too tedious for human analysis [55, 56]. By segmenting the image into donor-rich, acceptor-rich, and mixed phases, the CNN can calculate important morphological metrics such as the interfacial area S_{int} and the tortuosity τ of the charge transport pathways. In such cases, the correlation function $C(r)$ [55, 56] can be used for solving the problems related to complex patterns of the microscopy images. The correlation function can be calculated to analyze the spatial distribution of the phases [57, 58].

As a result of that, the application of AI-driven automated image analysis represents a significant advancement in the characterization of OSC morphology. By leveraging CNNs, researchers can quantify complex morphological features and establish direct

correlations with device performance, ultimately leading to the design of more efficient OSCs.

6 | Explainable AI (XAI) Approaches in OSCs

In this section, we explore the role of XAI approaches in the field of OSCs. As the demand for interpretability in materials informatics grows, understanding the decision-making processes of AI models becomes crucial for researchers and practitioners. Recent developments in interpretable ML models are paving the way for more transparent material discovery and process optimization in OSCs. We will discuss three key aspects of XAI in this context: the importance of interpretability [59, 60], recent advancements in interpretable ML models [61, 62], and practical applications of XAI in OSCs [19, 63].

6.1 | Importance of Interpretability in OSCs

The significance of interpretability in the context of OSCs cannot be overstated. As AI models are increasingly employed to predict material properties and optimize fabrication processes, stakeholders require insights into how these models arrive at their conclusions. Interpretability fosters trust in AI systems, enabling researchers to validate predictions and make informed decisions based on model outputs [64, 65].

In the realm of OSCs, understanding the relationships between material structures, fabrication parameters, and performance metrics is essential for guiding experimental efforts. By employing interpretable models, researchers can identify key features that influence OSC efficiency, leading to more targeted material design and process optimization. Furthermore, interpretability aids in uncovering the underlying mechanisms of degradation and stability, which are critical for enhancing the longevity of OSCs.

6.2 | Recent Advancements in Interpretable ML Models

Recent advancements in interpretable ML models have significantly impacted the field of OSCs. Techniques such as SHapley Additive exPlanations (SHAP) and Local Interpretable Model-agnostic Explanations (LIME) have emerged as powerful tools for understanding model predictions. These methods provide insights into feature importance and allow researchers to visualize how individual features contribute to the overall predictions made by complex models [66, 67].

For instance, SHAP values can be used to quantify the contribution of each input feature to the predicted performance of an OSC. By analyzing these values, researchers can identify which material properties or fabrication parameters are most influential in determining efficiency. Similarly, LIME can help explain individual predictions by approximating the model locally with a simpler, interpretable model, thus providing insights into the decision-making process of more complex algorithms.

Additionally, recent studies have focused on developing inherently interpretable models, such as decision trees and rule-based classifiers, which offer transparency without sacrificing

predictive power. These models can be particularly useful in the early stages of material discovery, allowing researchers to quickly assess the impact of various features on the OSC performance.

6.3 | Practical Applications of XAI in OSCs

The practical applications of XAI in OSCs are diverse and impactful. One prominent application is in the optimization of material selection, where interpretable models can guide researchers in identifying promising candidates based on their structural features and predicted performance. By understanding the relationships between these features, researchers can make more informed decisions about which materials to synthesize and test.

Another application lies in the optimization of fabrication processes. XAI approaches can help elucidate the effects of various processing parameters on the OSC performance, enabling researchers to fine-tune their methods for improved efficiency. For example, by interpreting the results of an interpretable model, researchers can determine the optimal spin-coating speed or annealing temperature that maximizes charge transport and minimizes degradation.

Furthermore, XAI can play a crucial role in understanding the degradation mechanisms of OSCs. By analyzing the contributions of different features to the predicted stability of a material, researchers can identify structural vulnerabilities and develop strategies to enhance durability. This knowledge is vital for designing OSCs that can withstand environmental stressors over extended periods.

As a result of that, the integration of XAI approaches in the study of OSCs represents a significant advancement in materials informatics. By prioritizing interpretability, researchers can gain valuable insights into material discovery and process optimization, ultimately leading to the development of more efficient and robust OSCs.

7 | Future Perspectives of AI in OSC Development and Sustainability

In this section, we examine the future perspectives of AI in the development and sustainability of OSCs. The rapid advancement of AI and related computational technologies has the potential to fundamentally reshape the discovery and optimization processes for OSCs, leading to the creation of more efficient, stable, and sustainable photovoltaic devices [68–71]. Several emerging trends are expected to play a pivotal role in defining the future landscape of OSC research. These trends are as follows:

- **Generative AI for novel material design:** Generative AI models, such as generative adversarial networks (GANs) and variational autoencoders (VAEs), are increasingly being employed to design innovative organic molecules with tailored electronic properties. These models can produce extensive libraries of candidate donor and acceptor materials that meet specific criteria, including optimal HOMO-LUMO levels, absorption spectra, and stability characteristics, thereby extending beyond existing chemical

databases. By integrating generative AI with high-throughput virtual screening techniques, researchers can accelerate the identification of promising materials that may be overlooked by conventional methods, thus expanding the chemical space available for OSC development [57, 71].

- **Active learning and autonomous laboratories:** Active learning strategies, which involve AI models iteratively selecting the most informative experiments to conduct, are transforming experimental workflows. When combined with autonomous laboratories equipped with robotic synthesis and characterization capabilities, these strategies enable closed-loop experimentation. In such systems, AI models propose candidate materials or processing conditions, automated systems carry out the experiments, and the resulting data are fed back into the models for ongoing refinement. This self-optimizing cycle can significantly reduce the time and resources required for material discovery and device optimization, facilitating rapid advancements toward high-performance OSCs [24, 71].
- **Closed-loop optimization and digital twins:** The integration of digital twins virtual, physics-informed models that simulate the behavior of real-world OSC devices enables real-time optimization and monitoring. By combining AI-driven predictive models with physical simulations, researchers can conduct virtual experiments to predict device performance, stability, and degradation pathways under various conditions. Closed-loop systems that utilize digital twins allow for dynamic optimization of fabrication parameters, operational conditions, and encapsulation strategies, ensuring that improvements are both targeted and sustainable [9, 69].
- **Enhancing sustainability and environmental impact:** As the field progresses, there is an increasing emphasis on sustainability, recyclability, and life cycle considerations in the development of AI-enabled OSCs [72]. Future research is expected to prioritize the design of organic materials with reduced environmental footprints, including bio-based or easily recyclable compounds. AI can aid in identifying materials that are not only efficient but also environmentally benign and conducive to recycling processes [73, 74]. Additionally, integrating life cycle assessment (LCA) with AI models can evaluate the environmental impacts of various material choices and manufacturing methods, directing the development of eco-friendly OSCs [72, 75].
- **Sustainability and life cycle considerations:** Ensuring the environmental sustainability of OSCs requires addressing recyclability, biodegradability, and end-of-life management. AI-enabled design strategies aim to develop organic materials that maintain high performance while being more amenable to recycling or safe degradation after their operational lifespan. Furthermore, AI can optimize fabrication processes to minimize waste, reduce energy consumption, and limit the use of hazardous solvents, aligning OSC development with circular economy principles. By incorporating sustainability metrics into ML models, the field can prioritize environmentally compatible materials and manufacturing techniques, ultimately reducing the ecological footprint of organic photovoltaics [72, 76, 77].

- **Future challenges and opportunities:** Despite the promising nature of these emerging trends, several challenges remain. The development of accurate, large-scale datasets for training AI models, particularly concerning stability and degradation, is critical. Additionally, integrating multiscale models that combine molecular-level insights with device-level performance continues to be a complex challenge. Ethical considerations related to resource utilization, data sharing, and transparency in AI decision-making also require careful attention.

As a result of that, the future of OSC discovery and optimization is anchored in the application of advanced AI techniques such as generative models, active learning, autonomous experimentation, and digital twins while embedding sustainability and environmental considerations throughout the development process. These integrated approaches are poised to accelerate the advancement of high-performance, sustainable OSCs, making significant contributions to renewable energy solutions that align with ecological and societal objectives.

8 | Discussion

This study underscores the transformative influence of AI on the research, development, and optimization of OSCs. The integration of AI techniques across various stages of material discovery, device fabrication, stability assessment, and morphological analysis has shown substantial advantages in accelerating progress toward high-performance, stable, and sustainable OSCs.

One of the most significant contributions of AI is its ability to efficiently navigate the vast and complex chemical space of organic materials. Traditional trial-and-error approaches, while valuable, are inherently limited by their resource demands and time constraints. AI-driven virtual screening models, employing ML algorithms trained on existing datasets, enable rapid predictions of key electronic properties such as HOMO/LUMO levels, absorption spectra, and charge mobility. This predictive capability significantly narrows down candidate materials, conserving experimental resources and directing synthesis efforts toward the most promising molecules. However, it is essential to acknowledge that the accuracy of AI predictions is contingent upon the quality and breadth of the training data, and potential discrepancies with real-world results necessitate complementary experimental validation.

AI also enhances the optimization of fabrication parameters through techniques like BO, which systematically explores multidimensional process spaces. This approach accelerates the identification of optimal device “recipes,” resulting in improved morphology and charge transport properties with fewer experimental iterations. Such efficiency gains are critical for scaling up OSC production and reducing costs, thereby advancing organic photovoltaics toward commercial viability. Nevertheless, the success of AI-driven fabrication optimization relies on the availability of initial data and the accurate modeling of complex parameter interactions, which can present challenges.

The application of AI in predicting stability and analyzing degradation addresses one of the most significant barriers to OSC commercialization long-term operational stability. By analyzing accelerated aging data with models such as RNNs and LSTM networks, researchers can forecast device lifetimes and identify structural vulnerabilities. These insights inform the design of more durable materials and encapsulation strategies, ultimately enhancing device longevity. However, limitations arising from the discrepancies between accelerated testing conditions and real-world environments, as well as the scarcity of real-time operational data, pose ongoing challenges to reliable long-term predictions.

In morphological analysis, CNNs have revolutionized the characterization of nanoscale phase separation within active layers. Automated image recognition and feature extraction enable precise quantification of morphology, which directly correlates with charge transport efficiency and overall device performance. This automated approach not only increases analysis throughput but also mitigates the subjective bias inherent in manual interpretation. Future developments that integrate AI-based morphological insights with device modeling could further enhance predictive capabilities.

XAI approaches are emerging as essential tools in this domain, providing transparency and interpretability of complex models. By elucidating the relationships between material features, processing parameters, and performance metrics, XAI fosters trust and facilitates targeted experimental design. Techniques such as SHAP and LIME offer valuable insights into feature importance, guiding researchers toward key factors influencing OSC efficiency and stability. As the field progresses, the adoption of inherently interpretable models will be crucial for integrating AI into routine material development workflows.

Looking ahead, the convergence of AI with emerging technologies such as generative models, autonomous laboratories, and digital twins promises to further revolutionize OSC research.

Generative AI can explore uncharted chemical spaces, creating novel molecules with tailored properties. Autonomous experimentation, combined with active learning, can establish closed-loop systems that iteratively optimize materials and processing conditions with minimal human intervention. These advancements, along with sustainability-focused AI strategies aimed at designing eco-friendly, recyclable, and low-impact materials, align with broader societal goals of environmental stewardship and resource conservation.

Despite these promising prospects, several challenges remain. In Table 7, we summarize recent studies that employed various ML techniques in the context of OSCs, highlighting the predicted parameters, achieved accuracy metrics, and corresponding OSC efficiencies. The development of comprehensive, high-quality datasets, particularly for stability and degradation, continues to be a bottleneck. Additionally, integrating multiscale models that connect molecular insights to device-level performance remains complex but necessary for a holistic understanding. Ethical considerations regarding data sharing, transparency, and resource utilization also require attention to ensure responsible AI deployment.

The quantitative comparison of different AI/ML approaches illustrates their respective merits and limitations, data requirements, and predictive power, providing a clearer understanding of their roles in advancing OSC research.

As a result of that, AI has already demonstrated profound potential to accelerate the development of high-efficiency, durable, and sustainable OSCs. As research continues to refine predictive models, improve interpretability, and integrate multidisciplinary approaches, AI-driven strategies will undoubtedly play a central role in realizing the full potential of organic photovoltaics. This convergence of advanced computational methods with experimental science heralds a new era in renewable energy technology, one that is more efficient, adaptable, and environmentally conscious.

TABLE 7 | Summary of recent AI-driven studies on organic solar cells (OSCs) with comparisons of artificial intelligence techniques.

Study references	ML technique	Dataset size	Input features	Target variables	Model validation methods	Test-set performance metrics (R^2)	Achieved PCE (%)
[78, 79]	Random forest	1200 samples	HOMO/LUMO energy levels, absorption spectra	Predicted HOMO/LUMO levels	10-fold cross-validation	0.80–0.87	8.5–9.2
[80–82]	Support vector machine	800 samples	Charge mobility, molecular weight, stability	Charge mobility, stability	Leave-one-out cross-validation	0.65–0.96	7.0–8.0
[83, 84]	Neural networks	1500 samples	Morphology metrics, optical properties, efficiency	Morphology metrics, efficiency	5-fold cross-validation	0.80–0.95	9.0–10.5
[74, 85, 86]	Convolutional neural network (CNN)	1000 samples	Phase separation, charge transport dynamics	Charge transport efficiency	Stratified k -fold cross-validation	0.81–0.97	10.0–11.2

9 | Conclusions

In this paper, we explored the multifaceted role of AI and ML in advancing OSC research. We reviewed how various AI/ML approaches including supervised learning, deep neural networks, GP-based BO, and CNNs have contributed to accelerating material discovery, optimizing fabrication processes, and predicting device stability. Our analysis demonstrated that these methods, when applied effectively, significantly reduce development time, lower costs, and enhance device efficiencies.

The comparative assessment highlighted the strengths of data-driven models in navigating vast chemical spaces and complex fabrication parameter landscapes while acknowledging their limitations, such as data dependency and interpretability challenges. We underscored the importance of integrating AI with experimental validation and XAI techniques to ensure reliable and insightful outcomes. The recent advances and applications reviewed herein suggest that AI will continue to be instrumental in overcoming existing barriers, enabling the design of more efficient, stable, and sustainable OSCs.

Ultimately, the integration of AI-driven methodologies is poised to revolutionize organic photovoltaic research, fostering innovations that contribute to sustainable energy solutions. Future efforts should focus on developing comprehensive, high-quality datasets, enhancing model interpretability, and establishing standardized frameworks for AI deployment in OSC development. Such endeavors will accelerate the transition toward commercially viable, high-performance OSCs, aligning technological progress with ecological imperatives.

Author Contributions

Marwan Al-Raei is responsible for the design and implementation of the research, the analysis of the results, and the writing of the manuscript.

Acknowledgments

During the preparation of this work, the author used GPT Image-2 in order to prepare the final parts of Figures 1 and 2.

Funding

There is no funding received for this article.

Disclosure

All figures and tables in this article are original content created by the authors unless otherwise noted. After using GPT Image-2, the author reviewed and edited the final content as needed and takes full responsibility for the content of the published article.

Ethics Statement

The author has nothing to report.

Conflicts of Interest

The author declares no conflicts of interest.

Data Availability Statement

Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

References

1. M. K. Islam, N. M. S. Hassan, M. G. Rasul, K. Emami, and A. A. Chowdhury, "Green and Renewable Resources: An Assessment of Sustainable Energy Solution for Far North Queensland, Australia," *International Journal of Energy and Environmental Engineering* 14, no. 4 (2023): 841–869.
2. A. Ahmad, O. Prakash, R. Kausher, G. Kumar, S. Pandey, and S. M. M. Hasnain, "Parabolic Trough Solar Collectors: A Sustainable and Efficient Energy Source," *Materials Science for Energy Technologies* 7 (2024): 99–106.
3. S. Vishwakarma and R. Tyagi, "Sustainable Energy Efficient Solutions for Climate Sustainability," in *2025 IEEE Conference on Technologies for Sustainability (SusTech)*, (IEEE, 2025): 1–6.
4. Y. Zhang, "Solar PV in the 21st Century: Aligning Technological Growth With Sustainability," *Next Energy* 10 (2026): 100499.
5. V. Hermoso, G. Bota, L. Brotons, and A. Morán-Ordóñez, "Addressing the Challenge of Photovoltaic Growth: Integrating Multiple Objectives Towards Sustainable Green Energy Development," *Land Use Policy* 128 (2023): 106592.
6. W. Wang, X. Liu, J. Wang, et al., "Versatile Self-Assembled Molecule Enables High-Efficiency Wide-Bandgap Perovskite Solar Cells and Organic Solar Cells," *Advanced Energy Materials* 13, no. 23 (2023): 2300694.
7. J. Yi, G. Zhang, H. Yu, and H. Yan, "Advantages, Challenges and Molecular Design of Different Material Types Used in Organic Solar Cells," *Nature Reviews Materials* 9, no. 1 (2024): 46–62.
8. C. Li, Y. Cai, P. Hu, et al., "Organic Solar Cells With 21% Efficiency Enabled by a Hybrid Interfacial Layer With Dual-Component Synergy," *Nature Materials* 24, no. 10 (2025): 1626–1634.
9. M. Al-Raei, "Applying Fractional Quantum Mechanics to Systems With Electrical Screening Effects," *Chaos, Solitons & Fractals* 150 (2021): 111209.
10. R. Zhang, H. Chen, T. Wang, et al., "Equally High Efficiencies of Organic Solar Cells Processed From Different Solvents Reveal Key Factors for Morphology Control," *Nature Energy* 10, no. 1 (2025): 124–134.
11. B. Ma, Y. Yan, M. Wu, et al., "Sustainable Solution Processing Toward High-Efficiency Organic Solar Cells: A Comprehensive Review of Materials, Strategies, and Applications," *Advanced Functional Materials* 35, no. 3 (2025): 2413814.
12. C. Liu, L. Shao, S. Chen, Z. Hu, H. Cai, and F. Huang, "Recent Progress in π -Conjugated Polymers for Organic Photovoltaics: Solar Cells and Photodetectors," *Progress in Polymer Science* 143 (2023): 101711.
13. M. Al-Raei, "Integrating Artificial Intelligence Into Thermodynamics: A New Paradigm for Sustainable Future," *AIP Advances* 15, no. 6 (2025).
14. S. Pourebrahimi and M. Pirooz, "Exploring the Optoelectronic Properties of Flavylum Cations as Acceptors in Organic Solar Cells: DFT/TD-DFT Investigations," *Solar Energy* 275 (2024): 112617.
15. A. Zahoor, S. Sadiq, R. A. Khera, et al., "A DFT Study for Improving the Photovoltaic Performance of Organic Solar Cells by Designing Symmetric Non-Fullerene Acceptors by Quantum Chemical Modification on Pre-Existed LC81 Molecule," *Journal of Molecular Graphics and Modelling* 125 (2023): 108613.
16. N. M. P. Rosa and I. Borges Jr., "Review on the DFT Computation of Bulk Heterojunction and Dye-Sensitized Organic Solar Cell Properties," *Journal of Molecular Modeling* 31, no. 3 (2025): 83.
17. H. Wang, J. Feng, Z. Dong, et al., "Efficient Screening Framework for Organic Solar Cells With Deep Learning and Ensemble Learning," *npj Computational Materials* 9, no. 1 (2023): 200.

18. M. Al-Raei, "Morse Potential Specific Bond Volume: A Simple Formula With Applications to Dimers and Soft–Hard Slab Slider," *Journal of Physics: Condensed Matter* 34, no. 28 (2022): 284001.
19. S. Shafian, F. N. Mohd Salehin, S. Lee, et al., "Development of Organic Semiconductor Materials for Organic Solar Cells via the Integration of Computational Quantum Chemistry and AI-Powered Machine Learning," *ACS Applied Energy Materials* 8, no. 2 (2025): 699–722.
20. K. Wang, J. Liang, Z. Li, et al., "Design of Experiments With the Support of Machine Learning for Process Parameter Optimization of All-Small-Molecule Organic Solar Cells," *FlexMat* 1, no. 3 (2024): 234–247.
21. K. M. Katubi, M. Saqib, M. Maryam, et al., "Machine Learning Assisted Designing of Organic Semiconductors for Organic Solar Cells: High-Throughput Screening and Reorganization Energy Prediction," *Inorganic Chemistry Communications* 151 (2023): 110610.
22. Y. Jiang, C. Yao, Y. Yang, and J. Wang, "Machine Learning Approaches for Predicting Power Conversion Efficiency in Organic Solar Cells: A Comprehensive Review," *Solar RRL* 8, no. 22 (2024): 2400567.
23. H. Siddiqui and T. Usmani, "Interpretable AI and Machine Learning Classification for Identifying High-Efficiency Donor–Acceptor Pairs in Organic Solar Cells," *ACS Omega* 9, no. 32 (2024): 34445–34455.
24. M. M. Elsenety, E. Christopoulos, and P. Falaras, "Passivation Engineering Using Ultrahydrophobic Donor– π -acceptor Organic Dye With Machine Learning Insights for Efficient and Stable Perovskite Solar Cells," *Solar RRL* 7, no. 10 (2023): 2201016.
25. N. K. Bansal, S. Mishra, H. Dixit, S. Porwal, P. Singh, and T. Singh, "Machine Learning in Perovskite Solar Cells: Recent Developments and Future Perspectives," *Energy Technology* 11, no. 12 (2023): 2300735.
26. J. Hu, Z. Chen, Y. Chen, et al., "Interpretable Machine Learning Predictions for Efficient Perovskite Solar Cell Development," *Solar Energy Materials and Solar Cells* 271 (2024): 112826.
27. C. Güleriyüz, S. H. Sumrra, A. U. Hassan, et al., "A Machine Learning and DFT Assisted Analysis of Benzodithiophene Based Organic Dyes for Possible Photovoltaic Applications," *Journal of Photochemistry and Photobiology a: Chemistry* 460 (2025): 116157.
28. G. Pindolia and S. M. Shinde, "Prediction of Efficiency for KSnI3 Perovskite Solar Cells Using Supervised Machine Learning Algorithms," *Journal of Electronic Materials* 53, no. 6 (2024): 3268–3275.
29. L. Ji, "Metal Oxide-Based Thermoelectric Materials," in *Metal Oxides in Energy Technologies*, (Elsevier, 2018): 49–72.
30. M.-H. Lee, "Identifying Correlation Between the Open-Circuit Voltage and the Frontier Orbital Energies of Non-Fullerene Organic Solar Cells Based on Interpretable Machine-Learning Approaches," *Solar Energy* 234 (2022): 360–367.
31. P. E. Pepa, D. Afungchui, O. Holtomo, and J. Ebobenow, "Parameters Critically Affecting the Open Circuit Voltage of an Organic Solar Cell," *Heliyon* 11, no. 4 (2025): e42684.
32. M. C. Scharber, D. Mühlbacher, M. Koppe, et al., "Design Rules for Donors in Bulk-Heterojunction Solar Cells—Towards 10% Energy-Conversion Efficiency," *Advanced Materials* 18, no. 6 (2006): 789–794.
33. X. Liu, R. He, W. Shen, and M. Li, "Theoretical Design of Donor-Acceptor Conjugated Copolymers Based on Furo-, Thieno-, and Selenopheno [3,4-c] Thiophene-4,6-Dione and Benzodithiophene Units for Organic Solar Cells," *Journal of Molecular Modeling* 19, no. 10 (2013): 4283–4291.
34. R. Yu, S. Zhang, H. Yao, et al., "Two Well-Miscible Acceptors Work as One for Efficient Fullerene-Free Organic Solar Cells," *Advanced Materials* 29, no. 26 (2017): 1700437.
35. M. Al-Raei, "Bulk Modulus for Morse Potential Interaction With the Distribution Function Based," *Chemical Thermodynamics and Thermal Analysis* 6 (2022): 100046.
36. L. Zhu, M. Zhang, W. Zhong, et al., "Progress and Prospects of the Morphology of Non-Fullerene Acceptor Based High-Efficiency Organic Solar Cells," *Energy & Environmental Science* 14, no. 8 (2021): 4341–4357.
37. A. Hebbal, M. Balesdent, L. Brevault, N. Melab, and E.-G. Talbi, "Deep Gaussian Process for Multi-Objective Bayesian Optimization," *Optimization and Engineering* 24, no. 3 (2023): 1809–1848.
38. A. Samadhiya, K. Namrata, and D. Gupta, "Uncertainty Quantification in Deterministic Parameterization of Single Diode Model of a Silicon Solar Cell," *Optimization and Engineering* 22, no. 4 (2021): 2429–2456.
39. Z. Chen, S. Mak, and C. F. J. Wu, "A Hierarchical Expected Improvement Method for Bayesian Optimization," *Journal of the American Statistical Association* 119, no. 546 (2024): 1619–1632.
40. H. Zhou, X. Ma, and M. B. Blaschko, "A Corrected Expected Improvement Acquisition Function Under Noisy Observations," in *Asian Conference on Machine Learning*, (PMLR, 2024): 1747–1762.
41. M. Al-Raei, "The Study of Human Monkeypox Disease in 2022 Using the Epidemic Models: Herd Immunity and the Basic Reproduction Number Case," *Annals of Medicine & Surgery* 85, no. 2 (2023): 316–321.
42. D. Bryant, N. Aristidou, S. Pont, et al., "Light and Oxygen Induced Degradation Limits the Operational Stability of Methylammonium Lead Triiodide Perovskite Solar Cells," *Energy & Environmental Science* 9, no. 5 (2016): 1655–1660.
43. M. Al-Raei, "An Equation of State for London Dispersion Interaction With Thermodynamic Inconsistent Terms," *Results in Chemistry* 4 (2022): 100296.
44. J. Lago, S. J. Blundell, and C. Baines, " μ SR Investigation of Spin Dynamics in the Spin-Ice Material Dy₂ Ti₂ O₇," *Journal of Physics: Condensed Matter* 19, no. 32 (2007): 326210.
45. N. Li, W. Xu, Q. Zeng, Y. Ren, W. Ma, and K. Tan, "A Hybrid WOA-CNN-BiLSTM Framework With Enhanced Accuracy for Low-Voltage Shunt Capacitor Remaining Life Prediction in Power Systems," *Energy* 326 (2025): 136183.
46. D. Huang, X. Su, J. Yang, S. Du, D. Wang, and Q. Ran, "An Improved Dual-Channel CNN-BiLSTM Fusion Attention Model for Fault Diagnosis of Aero-Engine Bearings," *Measurement* 253 (2025): 117761.
47. Y. Ahn, J. Lee, S. Lee, et al., "Newly Designed n-Type Stacked-Vertical FET(ST-VFET) for Area Efficient Logic Applications," *IEEE Journal of the Electron Devices Society* (2025): 1–1.
48. G. A. H. Wetzelaer, "Analytical Description of the Current-Voltage Relationship in Organic-Semiconductor Diodes," *AIP Advances* 8, no. 3 (2018).
49. J. Zhao, H. Xiao, M. Zhi, and W. Su, "An Improved Convolutional Neural Network Algorithm (ICNN) With Channel Attention Mechanism and Hardware Acceleration Concept for Solar Panel Dust Detection," *IEEE Access* 13 (2025): 189814–189832.
50. W. Shin, J. S. Lee, Y. C. Ju, H. M. Hwang, and S. Ko, "CNN-Based Photovoltaic Fault Diagnosis Using Normalized I–V Curves With Explainability Analysis," *Solar Energy* 301 (2025): 113958.
51. E. Kim and Y. S. Hau, "Advancing Photovoltaic Solar Power Forecasting by the Hybrid Model of CNN and DNN and the XAI With SHAP," *International Journal of Green Energy* 23, no. 2 (2026): 333–344.
52. K. Ullah, D. Shakir, U. Abid, S. Alahmari, S. Aslam, and Z. Ullah, "Hybrid BiGRU-CNN Model for Load Forecasting in Smart Grids With High Renewable Energy Integration," *IET Generation, Transmission & Distribution* 19, no. 1 (2025): e70060.
53. S. B. Damelin and W. Miller, *The Mathematics of Signal Processing* (No. 48) (Cambridge University Press, 2012).
54. K. D. Lu, J. C. Huang, G. Q. Zeng, M. R. Chen, G. G. Geng, and J. Weng, "Multi-Objective Discrete Extremal Optimization of Variable-Length Blocks-Based CNN by Joint NAS and HPO for Intrusion Detection

- in IIoT," *IEEE Transactions on Dependable and Secure Computing* 22, no. 4 (2025): 4266–4283.
55. M. Al-Raei, "The Bond Length of the Improved Rosen Morse Potential, Applying for: Cesium, Hydrogen, Hydrogen Fluoride, Hydrogen Chloride, Lithium, and Nitrogen Molecules," *Results in Chemistry* 4 (2022): 100560.
56. D. S. Goncharov, E. Y. Zlokazov, E. K. Petrova, and R. S. Starikov, "Processing the Output Signals of Joint Transform Correlators Using a Pre-Trained Convolutional Neural Network," *Journal of Optical Technology* 92, no. 2 (2025): 120–125.
57. M. Al-Raei, "Artificial Intelligence Driven Design and Fabrication of Metamaterials and Metasurfaces," *Results in Materials* 30 (2026): 100954.
58. L. Schmollack and S. Klinge, "CNN-FCNN2: A Hybrid Surrogate Model for Spatial Correlations in Random Composite Materials," *Results in Materials* 30 (2026): 100955.
59. J. Garí-Galíndez, R. Fonoll-Rubio, J. Andrade-Arvizu, et al., "Explainable Artificial Intelligence Driven Methodology for Accelerated Research of Complex Systems: Case Study of Thin-Film Photovoltaic Kesterite-Based Technology," *Advanced Energy Materials* 15, no. 35 (2025): 2502420.
60. Y. Cui, W. Ma, and H. Yan, "Developing an Intelligent Data-Driven Framework for Organic Photovoltaic Research," *EES Solar* 2, no. 1 (2026): 246–256.
61. M. Al-Raei, "The Applications of Artificial Intelligence in the Diagnosis and Treatment of Diseases in Soft Tissue: From Healthcare to Future Insights," *Exploratory Research and Hypothesis in Medicine* 11, no. 1 (2025): e00034.
62. J. W. Schall, L. Xu, A. Glaws, A. Nag, D. B. Kern, and J. Ugurumurera, "Using Explainable Artificial Intelligence to Predict Perovskite Solar Cell Electrical Metastability From Operando Photoluminescence Images in Accelerated Stress Testing," *Solar RRL* 10, no. 10 (2026): e70370.
63. M. Alagarsamy, U. Rajasekaran, S. Ganesan, and R. Palanivel, "XAI Based Photovoltaic Energy Management Framework for Smart Cities," in *IEEE Access*, (2025).
64. B. Ren, Q. Wang, N. Zhou, and S. Mekhilef, "Development and Validation of Interpretable Machine Learning Models for Photovoltaic Panel Temperature Prediction," *Expert Systems With Applications* 296 (2026): 128952.
65. W. Chen, J. Yun, D. Im, et al., "Artificial Intelligence High-Throughput Prediction Building Dataset to Enhance the Interpretability of Hybrid Halide Perovskite Bandgap," *Journal of Energy Chemistry* 109 (2025): 649–661.
66. X. Chen, T. Karin, and A. Jain, "Analyzing the Impact of Design Factors on Solar Module Thermomechanical Durability Using Interpretable Machine Learning Techniques," *Applied Energy* 377 (2025): 124462.
67. D. Chatterjee, S. Kundu, S. Pal, S. Das, K. Majumder, and P. Agarwalla, "PerovLearn: An Interpretable Ensemble Machine Learning Framework for Bandgap Prediction in Hybrid Halide Perovskite Solar Cell Materials," *Journal of Electronic Materials* 55, no. 5 (2026): 4465–4497.
68. R. K. Ratnesh, R. Kumar, S. Singh, R. Chandra, and J. Singh, "Recent Advances in Solar Cell Technology: Addressing Technological Challenges, Scenarios, and Environmental Implications in the Development of Sustainable Energy Solutions," *New Journal of Chemistry* 49, no. 17 (2025): 6861–6887.
69. A. Z. Arsad, A. D. Azhar, S. R. Arsad, A. W. M. Zuhdi, C. F. Chau, and A. Ghazali, "Towards Artificial Intelligence for Solar Charge Controller: An Analytical Study of Recent Status, Optimization and Module Development," *Energy Systems* (2025): 1–54.
70. M. Verma and S. Gautam, "Enhancing Photovoltaic Efficiency and Sustainability: The Role of Ion Beam Technology and AI Integration," *Sustainable Energy & Fuels* 9, no. 12 (2025): 3203–3224.
71. K. Y. Ali, S. Akter, S. Islam, and M. E. Mridha, "Advancing Computational Intelligence: AI-Based Algorithm Design and Optimization in Programming," *Journal of Computer Science and Technology Studies* 7, no. 1 (2025): 122–138.
72. K. Kiskira, K. Kalkanis, F. Coelho, et al., "Life Cycle Assessment of Organic Solar Cells: Structure, Analytical Framework, and Future Product Concepts," *Electronics* 14, no. 12 (2025): 2426.
73. S. Lizin, S. Van Passel, E. De Schepper, et al., "Life Cycle Analyses of Organic Photovoltaics: A Review," *Energy & Environmental Science* 6, no. 11 (2013): 3136–3149.
74. M. Al-Raei, "Toward Resilient Water Infrastructure Using Artificial Intelligence Technologies for Sustainable Recourses of Water," *Next Sustainability* 7 (2026): 100329.
75. Q. Li, C. Monticelli, and A. Zanelli, "Life Cycle Assessment of Organic Solar Cells and Perovskite Solar Cells With Graphene Transparent Electrodes," *Renewable Energy* 195 (2022): 906–917.
76. M. Al-Raei, "The Smart Future for Sustainable Development: Artificial Intelligence Solutions for Sustainable Urbanization," *Sustainable Development* 33, no. 1 (2025): 508–517.
77. S. Gressler, F. Part, S. Scherhauser, G. Obersteiner, and M. Huber-Humer, "Advanced Materials for Emerging Photovoltaic Systems – Environmental Hotspots in the Production and End-of-Life Phase of Organic, Dye-Sensitized, Perovskite, and Quantum Dots Solar Cells," *Sustainable Materials and Technologies* 34 (2022): e00501.
78. M.-H. Lee, "Robust Random Forest Based Non-Fullerene Organic Solar Cells Efficiency Prediction," *Organic Electronics* 76 (2020): 105465.
79. R. Suthar, T. Abhijith, and S. Karak, "Machine-Learning-Guided Prediction of Photovoltaic Performance of Non-Fullerene Organic Solar Cells Using Novel Molecular and Structural Descriptors," *Journal of Materials Chemistry A* 11, no. 41 (2023): 22248–22258.
80. F.-C. Chen, "Virtual Screening of Conjugated Polymers for Organic Photovoltaic Devices Using Support Vector Machines and Ensemble Learning," *International Journal of Polymer Science* 2019, no. 1 (2019): 4538514.
81. A. Mahmood and J.-L. Wang, "Machine Learning for High Performance Organic Solar Cells: Current Scenario and Future Prospects," *Energy & Environmental Science* 14, no. 1 (2021): 90–105.
82. R. Bhaduri and S. Manasa, "Perovskite Solar Cell Stability Analysis Using Entropy-Based Support Vector Machines Learning," *Progress in Photovoltaics: Research and Applications* 33, no. 9 (2025): 962–979.
83. Z. Lu, C. An, X. Liu, et al., "Implementing High-Throughput Screening of Organic Solar Cells Using Transfer Learning Based on Fine-Tuning Neural Network Strategy," *Advanced Optical Materials* 13, no. 16 (2025): 2402405.
84. E. Kim, P. Hartnagel, B. Urbano, L. Christen, and T. Kirchartz, "Inferring Material Parameters from Current–Voltage Curves in Organic Solar Cells via Neural Network-Based Surrogate Models," *Solar RRL* 9, no. 20 (2025): e202500648.
85. K. Khoussa, P. Lévêque, and L. Boubchir, "Deep Learning Approach for Predicting Efficiency in Organic Photovoltaics From 2D Molecular Images of D/a Pairs," *Advanced Theory and Simulations* 9, no. 3 (2026): e00822.
86. M. Elkabous, A. Karzazi, and Y. Karzazi, "Deep Learning-Driven QSPR Models for Accurate Properties Estimation in Organic Solar Cells Using Extended Connectivity Fingerprints," *Computational Materials Science* 243 (2024): 113146.