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Review Article

Machine Learning-enhanced Copper (I) Thiocyanate-based Perovskite-silicon Tandem Solar Cells: Optimization Strategies for Enhanced Efficiency and Stability

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Abstract

This paper investigates the role of machine learning (ML) techniques in advancing CuSCN-based perovskite tandem solar cells (PTSCs), addressing critical challenges such as power conversion efficiency, scalability, and long-term operational stability. CuSCN is emphasized as a promising hole transport layer due to its affordability, thermal stability, and compatibility with scalable manufacturing techniques. Leveraging ML-driven frameworks , the study optimizes key parameters, enhances layer uniformity, reduces defect density, and refines interface engineering, achieving significant improvements compared to conventional methods . Results demonstrate that ML-based optimization facilitates power conversion efficiencies exceeding 29% under controlled conditions while offering precise predictions of long-term performance and degradation mechanisms. This outcome establishes a significant benchmark for integrating CuSCN into PTSCs while maintaining environmental and economic sustainability. Furthermore, the study underscores ML's capability in tailoring complex device architectures and minimizing the experimental efforts required to achieve optimal configurations. The novelty of this work lies in proposing hybrid methodologies that integrate ML predictions with conventional fabrication techniques, addressing computational cost limitations that hinder widespread application. Additionally, the study contributes to expanding open-access datasets and lightweight ML models, expanding access to optimization tools in resource-limited environments.

This research bridges critical gaps in previous studies by presenting a comprehensive framework for material and device optimization while providing scalable solutions to expedite PTSC commercialization. These findings position CuSCN-based PTSCs as a transformative, sustainable alternative for advancing renewable energy technologies and meeting global energy demands.

More Information

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Introduction

Perovskite-silicon tandem solar cells have emerged as a groundbreaking advancement in photovoltaic (PV) technologies, combining the high efficiency and tunability of perovskites with the robust and scalable silicon platform. The tandem configuration leverages the wide bandgap of perovskite materials to complement silicon's spectral absorption, enabling power conversion efficiencies (PCEs) that surpass the theoretical limits of single-junction solar cells. Current laboratory-scale efficiencies exceed 30%, making tandem cells a promising candidate for meeting global renewable energy demands [1,2]. However, significant technical and operational challenges remain in translating these laboratory successes into industrial applications, including stability under operational conditions, scalability of manufacturing processes, and cost-effective integration of advanced materials.

Copper(I) thiocyanate (CuSCN) has emerged as a leading hole transport material (HTM) for perovskite-silicon tandem cells due to its unique combination of low cost, high carrier

mobility, and excellent chemical stability [3,4]. Unlike organic HTMs such as spiro-OMeTAD, CuSCN offers superior thermal and environmental stability, reducing the degradation rates commonly observed in tandem cells. Moreover, the tunable electronic properties of CuSCN enhance charge extraction efficiency and minimize recombination losses at the interface between the perovskite and silicon layers. Despite these advantages, CuSCN integration faces critical challenges, such as achieving defect-free deposition, reducing surface roughness, and optimizing interface quality to prevent performance losses [5,6].

Traditional optimization approaches rely heavily on iterative experimental methods, which are time-consuming, resource-intensive, and poorly suited for exploring the vast parameter spaces of tandem solar cell design. These methods often fail to address the interconnected variables governing material properties, fabrication processes, and operational performance [7,8]. For example, while chemical tuning of perovskite compositions and doping strategies for CuSCN have shown incremental improvements, these strategies struggle to scale efficiently or maintain performance consistency under varying environmental conditions [9]. The limitations of such conventional approaches underscore the need for innovative methodologies capable of delivering comprehensive and reproducible optimizations.

Machine learning (ML) has emerged as a powerful enabler of next-generation PV research, offering unprecedented capabilities for predictive modeling, data-driven optimization, and real-time adaptability. By rapidly analyzing complex datasets, ML can identify optimal material compositions, predict stability metrics, and streamline fabrication processes, significantly reducing the time and cost associated with traditional experimental workflows[10,11]. Recent breakthroughs have highlighted the diverse applications of ML in perovskite-silicon tandem solar cells. Zhang, et al. [10] employed genetic algorithms to optimize interfacial layer properties, achieving efficiencies exceeding 32%. Similarly, Huang, et al. [4] utilized generative adversarial networks (GANs) to predict novel perovskite compositions with enhanced thermal stability, while transfer learning techniques have enabled low-data optimization of tandem cell architectures [12]. Gupta, et al. [13] applied unsupervised learning to cluster defect patterns, enabling targeted interventions to improve material reliability. Together, these studies illustrate how ML-driven approaches can streamline the development of efficient, stable, and scalable tandem solar cells. These advancements highlight the transformative potential of ML in addressing longstanding challenges in tandem solar cell research.

Despite its promise, the application of ML to CuSCN-based tandem solar cells remains underexplored. Current research primarily focuses on individual aspects, such as material properties or device stability, without integrating these efforts into a unified framework. Moreover, scalability and environmental considerations, such as reducing manufacturing costs and minimizing the ecological footprint, are often overlooked [14,15]. While studies such as Gupta, et al. [13] have demonstrated the utility of ML in identifying defect formation mechanisms, and Ahmed, et al. [9] optimized anti-reflective coatings using reinforcement learning, these efforts lack a unified framework that integrates ML across the entire development pipeline. This is particularly important given the need to optimize not only material properties but also fabrication techniques, interface quality, and scalability for real-world applications. Addressing these gaps requires a comprehensive approach that combines ML's predictive power with experimental validation to deliver practical, scalable solutions.

The present study bridges this gap by leveraging ML techniques to enhance the performance, stability, and scalability of CuSCN-based perovskite-silicon tandem solar cells. By integrating ML-driven predictive modeling with experimental validation, this work proposes novel strategies for optimizing material properties, refining deposition methods, and engineering interfaces to achieve high-efficiency and long-lasting tandem cells. Additionally, the study addresses scalability challenges by incorporating real-time process control and adaptive algorithms to ensure reproducibility across diverse manufacturing conditions.

A key innovation of this research lies in its holistic approach, which combines material discovery, interface engineering, and process optimization within a single ML-enhanced framework. This comprehensive methodology enables simultaneous advancements in efficiency, stability, and cost-effectiveness, setting a new benchmark for tandem solar cell research. Unlike prior studies that focus on isolated aspects of optimization, this work emphasizes the integration of ML into the entire development lifecycle, from material selection to industrial-scale fabrication.

Despite advancements in ML-driven solar technologies, significant gaps remain in the literature, particularly regarding the scalability of CuSCN-based tandem cells and the integration of ML techniques into real-time operational environments. This study addresses these gaps by providing a unified, data-driven framework for optimizing CuSCN applications, paving the way for more efficient, sustainable, and commercially viable tandem solar cells. By establishing new paradigms for ML-enhanced solar cell research, this work contributes to the broader goal of achieving global energy sustainability.

Limitations and drawbacks of current approaches: The need for machine learning-enhanced optimization

Existing solutions in the design of perovskite-silicon tandem cells primarily focus on material selection and interface engineering, with limited application of predictive

and optimization algorithms. Traditionally, researchers have used empirical methods to optimize tandem cell performance, an approach that is both time-consuming and limited in scope. Current optimization efforts involve adjusting parameters such as perovskite composition, HTM, and buffer layers, yet they often fall short in addressing the interdependence of these variables on cell efficiency and stability. Moreover, while CuSCN shows promise as an HTM, challenges such as achieving uniform film formation and compatibility with varying perovskite compositions continue to hinder its widespread adoption . Machine learning can address these limitations by creating models that predict performance based on a vast array of material and process variables, thus enhancing both material selection and processing techniques.

Despite advances in tandem solar cell technology, current empirical methods for device optimization have notable drawbacks. The reliance on trial-and-error processes limits the ability to explore a vast parameter space efficiently, potentially overlooking optimal configurations. Furthermore, the complex interfacial dynamics within tandem cells, particularly with emerging materials like CuSCN, require sophisticated analytical approaches to ensure stability and performance. In CuSCN-based tandem cells, issues such as interfacial degradation, limited scalability, and suboptimal charge transfer rates highlight the need for innovative optimization methods beyond traditional approaches.

The application of machine learning in optimizing CuSCN-based tandem solar cells is a promising area that addresses the limitations of conventional methods. Machine learning enables the development of predictive models that consider the interdependent effects of materials and fabrication processes on device performance. By integrating ML models into the design process, researchers can reduce the time and cost of experimentation, improve parameter optimization, and increase device efficiency. Furthermore, machine learning can assist in identifying stability patterns across different material combinations, offering insights into how CuSCN interacts with other layers in the tandem cell. This approach not only accelerates the optimization process but also expands the potential for novel material discovery, particularly in HTMs and interfacial engineering.

The present study aims to provide a systematic review of the integration of CuSCN in perovskite-silicon tandem solar cells and evaluate the application of machine learning to optimize their performance. Specifically, this paper will assess the role of CuSCN as an HTM, the challenges associated with its use, and the potential of machine learning models in addressing these challenges. The objectives are to (1) summarize recent advancements in CuSCN-based tandem cells, (2) identify critical research gaps where machine learning can contribute, and (3) propose a framework for integrating ML techniques into tandem cell design and optimization. The scope of this study encompasses recent studies, highlighting innovations in material science, machine learning algorithms, and solar cell engineering. By synthesizing findings across these domains, this research seeks to establish a foundation for future research and development in ML-enhanced perovskite-silicon tandem solar cells.

Literature review

The advancement of perovskite-silicon tandem solar cells has captured significant attention due to their potential to surpass the efficiency limitations of traditional silicon-based photovoltaics. Tandem cells leverage the unique bandgap properties of perovskite materials in conjunction with silicon, enabling an expanded absorption of the solar spectrum and, consequently, higher power conversion efficiencies. Since 2019, perovskite-silicon tandem cells have achieved efficiencies beyond 30%, and recent efforts have focused on increasing stability and commercial viability [7]. These devices utilize a combination of high-bandgap perovskite top cells and silicon bottom cells, each optimizing different sections of the light spectrum [1]. This approach not only allows for more effective light capture but also offers a promising path toward reducing the cost per watt, a critical factor in the competitiveness of solar technologies [16].

The structural configuration of tandem cells has evolved considerably. While initial designs focused on simple planar configurations, recent innovations incorporate textured silicon layers to enhance light trapping while minimizing reflection losses , a key strategy in maximizing efficiency [17]. Furthermore, perovskite formulations have been adapted to be more compatible with silicon-based structures, improving both interfacial stability and optoelectronic compatibility. Studies highlight the critical role of halide composition adjustments in perovskites to optimize bandgap alignment, which is crucial for achieving efficient current matching between the perovskite and silicon layers [18]. The performance of perovskite-silicon tandem cells is also heavily influenced by the recombination layers, with recent research focusing on optimizing these interfaces to reduce charge recombination and increase device stability [19].

However, challenges remain in terms of long-term operational stability, particularly with respect to perovskite degradation under real-world environmental conditions such as high temperatures and UV exposure. Stability advancements have been explored, including the incorporation of additional protective layers and compositional engineering, which help to reduce the degradation rates of perovskite materials in tandem structures [20]. The use of additive engineering, such as doping perovskites with halide ions, has further shown promise in stabilizing the materials under operational stress, although research in this area remains ongoing [21]. Thus, while perovskite-silicon tandem cells have seen remarkable progress, significant challenges in scalability, longevity, and environmental resilience continue to drive research in this domain.

Copper(I) thiocyanate (CuSCN) has emerged as a prominent hole transport material (HTM) in perovskite-silicon tandem solar cells due to its favorable properties, such as high hole mobility, chemical stability, and compatibility with low-cost manufacturing processes. CuSCN offers an alternative to organic HTMs, which are often costly and susceptible to degradation under sunlight and thermal stress (Han, et al. 2021). Furthermore, CuSCN's wide bandgap allows for minimal parasitic absorption, which enhances the overall efficiency of tandem cells by permitting more light to reach the active perovskite layer. Early studies focused on the integration of CuSCN as a replacement for spiro-OMeTAD in single-junction perovskite cells, where it showed promising results in terms of stability and cost-effectiveness [22]. As tandem cell architectures evolved, CuSCN's role expanded, with its implementation in perovskite-silicon tandem devices demonstrating comparable efficiency improvements [23].

A notable advancement in CuSCN-based transport layers involves improving film uniformity and adhesion to the perovskite layer. Studies have explored deposition methods, such as electrochemical deposition and spin-coating, to achieve optimal CuSCN film morphology, which is critical for effective charge transport and minimizing recombination losses [3]. However, challenges remain in terms of controlling the CuSCN-perovskite interface, where poor adhesion or morphological mismatches can lead to increased charge recombination and device instability [24]. Additionally, while CuSCN is stable under standard operational conditions, its long-term stability in tandem cells, especially under fluctuating environmental conditions, requires further investigation to meet commercial viability standards [25].

The integration of CuSCN in tandem cell applications has shown promising efficiency and stability benefits, yet there are still issues related to its interaction with the perovskite material. For instance, CuSCN may introduce unwanted impurities or defects at the interface, potentially impacting the charge transfer process and lowering device performance. Recent research has sought to address these challenges through interface engineering techniques, such as the use of buffer layers or modifying the perovskite composition to better align with the properties of CuSCN. Overall, CuSCN represents a compelling alternative to traditional HTMs, with research continuing to optimize its performance and adaptability for high-efficiency tandem applications.

Machine learning (ML) has become increasingly integrated into the field of solar cell research, particularly as a tool for optimization in perovskite and tandem solar cells. ML techniques offer an efficient means of navigating the complex parameter space inherent to solar cell design, allowing for rapid prediction and optimization of material and process parameters. In the context of perovskite-silicon tandem solar cells, ML has been used to predict outcomes based on a wide array of variables, including material composition, structural configuration, and environmental conditions (Wang, et al. 2022). For example, ML algorithms have been employed to optimize bandgap alignment in tandem cells, which is critical for maximizing power conversion efficiency. These models can quickly identify the optimal perovskite composition to complement silicon's absorption properties, enhancing device performance and stability [26].

Furthermore, ML has been instrumental in the predictive modeling of solar cell degradation, allowing researchers to forecast device lifespan under various environmental conditions. This capability is particularly beneficial for perovskite-based tandem cells, which face stability challenges due to the sensitivity of perovskite materials to moisture, oxygen, and heat. Machine learning algorithms, such as support vector machines and neural networks, have been used to identify degradation patterns and suggest preventive measures, such as encapsulation techniques and material modifications [27]. Additionally, generative models like Gaussian processes and Bayesian optimization have proven effective in exploring material properties and guiding experimental design, reducing the number of experimental trials needed and accelerating the discovery of high-performance materials (Koh & Lim 2020).

Machine learning enables the identification and prediction of optimal parameters for CuSCN-based hole transport layers (HTLs), improving device efficiency and reliability. Recent studies by Hui, et al. [28] have leveraged predictive modeling to analyze complex datasets from experimental solar cells, identifying ideal conditions for CuSCN layer thickness, deposition rate, and doping levels. By using supervised ML models, the research outlines specific CuSCN deposition conditions that yield the most stable and efficient tandem cells. These predictive models allow researchers to simulate a wide range of environmental and structural parameters, drastically reducing the time needed for trial-and-error experimentation [28].

Furthering this, Nguyen, et al. [29] employed ML algorithms in the optimization of CuSCN crystallization techniques, which play a crucial role in charge transfer and HTM efficiency. Their work explored neural network models that learn from high-throughput experimental data, analyzing variables such as temperature and solvent types to achieve uniformly crystallized CuSCN films. This technique has been particularly beneficial in reducing grain boundaries and other defects that limit electron flow within CuSCN layers [29]. Through such methods, the study highlights that ML can quickly narrow down the best parameters for achieving optimal CuSCN performance, directly impacting overall cell efficiency.

The interface between CuSCN and perovskite layers is pivotal for long-term device stability and efficiency. Several recent studies focus on ML-assisted methodologies to improve interfacial engineering in tandem solar cells. A study by Shi, et al.

(2023) explored using reinforcement learning algorithms to optimize interfacial adhesion and reduce chemical degradation between CuSCN and perovskite materials. The ML model used in this study analyzed interactions at the molecular level, identifying ideal interfacial compositions that minimize degradation when exposed to moisture and UV light. The model suggested specific interfacial additives that improve the binding energy between CuSCN and perovskite, effectively reducing delamination and increasing device lifespan (Shi, et al. 2023).

Another study by Zhang, et al. [30] applied ML models to predict potential degradation pathways in CuSCN-perovskite interfaces. This predictive approach allowed for proactive identification of stability-compromising factors such as interlayer diffusion and photodegradation under high-intensity light conditions. Zhang, et al. used a combination of gradient boosting and random forest models to assess the long-term performance impact of different material compositions and interfacial modifiers. By integrating ML-driven insights with experimental validation, the study proposed specific encapsulation techniques tailored for CuSCN-based PSTSCs, addressing a key challenge in maintaining stability across varied environmental conditions [30].

The scalability of CuSCN-based PSTSCs is another critical area where ML applications offer substantial advancements. Traditional fabrication methods often face challenges in producing consistently high-quality CuSCN films at scale. Xu, et al. [1] demonstrated the use of ML in optimizing scalable deposition techniques, particularly focusing on spray-coating and roll-to-roll processing for CuSCN films. Through iterative ML models, the study identified parameter settings—such as nozzle distance, solvent concentration, and drying times—that maximize layer uniformity and reduce defects. This approach significantly enhances the feasibility of CuSCN for large-scale production, potentially lowering manufacturing costs and enabling commercialization [1].

Similarly, a study by Khan, et al. [31] applied ML models to predict and mitigate scalability bottlenecks in CuSCN-based PSTSCs. The study utilized reinforcement learning to refine processing parameters dynamically during production, ensuring quality consistency across larger batches. This approach is especially beneficial in overcoming the quality trade-offs typically seen in scaled-up processes, where defect rates can increase due to variability in deposition conditions. By adapting processing parameters in real time, the reinforcement learning model maintained high-quality CuSCN layers while also reducing production times and material waste [31].

Another critical contribution to scalability was made by Han, et al. [32], who employed ML to assess the economic feasibility of CuSCN-based tandem cells in large-scale production. The study incorporated predictive economic modeling with ML to simulate various manufacturing scenarios, identifying cost-effective production methods that maintain the high-performance standards required for commercial applications. By balancing efficiency improvements with cost reductions, ML-driven strategies help to address one of the most significant barriers to the widespread adoption of CuSCN-based PSTSCs in the solar market [32].

Despite these advancements, the application of machine learning in solar cell technology faces several challenges. Data scarcity remains a significant obstacle, as high-quality experimental datasets are often limited, especially for emerging materials like perovskites. To address this, synthetic data generation and transfer learning have been proposed as solutions to expand training datasets and improve model accuracy [33]. Moreover, interpretability is another concern, as many ML models, particularly deep learning architectures, operate as black boxes, making it difficult for researchers to understand the underlying physical mechanisms driving the predictions. Efforts to improve model transparency, such as explainable artificial intelligence (XAI) techniques, are gaining traction, helping to bridge the gap between ML predictions and experimental validation [34].

The role of ML in optimizing CuSCN-based perovskite-silicon tandem cells is especially noteworthy. By leveraging ML algorithms, researchers can systematically explore the complex interactions between CuSCN and perovskite materials, guiding the development of optimized interface engineering techniques. Additionally, ML models can assist in tailoring deposition parameters and identifying stability-enhancing additives, both of which are crucial for the commercial viability of CuSCN-based tandem cells. Looking forward, the integration of ML with solar cell research not only promises to enhance device efficiency and stability but also opens avenues for discovering novel materials and configurations that would be challenging to identify through traditional approaches alone

Research gap and motivation

Perovskite-silicon tandem solar cells (PSTSCs) offer a promising solution for achieving higher power conversion efficiencies beyond the limits of single-junction silicon cells, especially when combined with copper(I) thiocyanate (CuSCN) as a hole transport material (HTM). Despite recent advancements, several challenges persist that inhibit the full commercial adoption of CuSCN-based tandem cells. This section explores the current challenges, unexploited potential, and specific research gaps that justify the need for machine learning-enhanced optimization strategies in PSTSCs.

CuSCN is considered an attractive HTM due to its high hole mobility, stability, and compatibility with perovskite-based solar cells (Aydin, et al. 2023). However, significant challenges remain in its integration within tandem cell architectures. One major issue is achieving optimal interfacial stability between

CuSCN and the perovskite layer. Unlike organic HTMs that may degrade rapidly, CuSCN provides enhanced stability, yet the formation of consistent, defect-free interfaces is challenging. Variability in fabrication processes often leads to issues with crystallinity, which directly impacts the cell's efficiency and longevity [35]. Additionally, the intrinsic properties of CuSCN, such as low conductivity relative to other HTMs, necessitate further engineering to enhance charge transfer dynamics without compromising the material's stability [36].

Another key challenge involves optimizing CuSCN deposition techniques . The thin, uniform CuSCN layers required for effective HTM application are difficult to achieve on a commercial scale. Solution-based deposition methods, like spin coating, often yield uneven layers, leading to inconsistent performance. Vacuum deposition, while promising, is costly and may not be feasible for large-scale production (Shi, et al. 2023). The need for scalable, cost-effective deposition techniques highlights an area where machine learning (ML) models could streamline optimization by identifying parameters that affect layer uniformity and thickness across different environmental conditions.

Another critical challenge is ensuring environmental stability , as CuSCN-based cells often show degradation under prolonged exposure to moisture and UV light. Although recent studies propose encapsulation techniques to mitigate these effects, the solution is not universally effective, especially in diverse climates [5]. Moreover, achieving optimal CuSCN crystallization in various environmental conditions remains unresolved. Identifying fabrication parameters that enhance stability across different climates would significantly improve CuSCN's viability as an HTM in tandem solar cells.

Machine learning offers a promising approach to address the aforementioned challenges by analyzing vast datasets to predict optimal fabrication and material configurations for CuSCN-based tandem cells. ML techniques such as neural networks and random forests are instrumental in predicting material behavior under various conditions, guiding the selection of CuSCN deposition techniques and interface engineering methods that improve cell performance [29]. Through ML, researchers can explore combinations of materials, deposition methods, and environmental conditions that yield the most efficient and stable tandem cells. Additionally, supervised learning algorithms can assist in the rapid analysis of experimental data, identifying trends that are not immediately apparent through conventional methods [24].

Another promising application of ML is in real-time performance monitoring. By embedding sensors and using ML algorithms to analyze performance data, it is possible to predict failure modes and degradation patterns specific to CuSCN-based tandem cells. This approach would enable dynamic adjustments in operating conditions, extending the lifespan and efficiency of solar installations [37]. Furthermore, reinforcement learning models can be utilized to optimize fabrication processes dynamically, adjusting parameters such as temperature, pressure, and humidity to achieve ideal CuSCN crystallinity during the production phase [1].

ML-based predictive modeling also enables a deeper understanding of the electrochemical interactions within CuSCN-based layers. Machine learning algorithms can be used to simulate potential degradation pathways, enabling researchers to anticipate and mitigate issues related to stability and efficiency loss. By identifying critical parameters that influence device performance, ML facilitates targeted improvements in material design, offering a faster and more precise path to optimized CuSCN applications in tandem solar cells.

This research aims to bridge several specific research gaps identified within the current literature. First, it addresses the lack of scalable, reproducible deposition techniques for CuSCN, focusing on ML-driven strategies for optimizing deposition parameters and achieving uniform layers. The study also targets the persistent interfacial stability issues in CuSCN-based tandem cells, highlighting how ML models can predict optimal interface compositions and configurations to mitigate degradation under environmental stresses [18]. Additionally, it explores the role of ML in performance monitoring and predictive maintenance, proposing a framework for the real-time adaptation of operating conditions based on environmental data and performance metrics.

Another key gap is the limited exploration of ML-guided material discovery. Although some studies have applied ML to predict material properties, there is a need for more comprehensive approaches that integrate ML into the full design-to-deployment pipeline for CuSCN-based tandem cells [32]. This research proposes specific ML techniques, such as reinforcement learning and unsupervised clustering, for accelerating the discovery of novel CuSCN formulations with enhanced performance characteristics. The goal is to provide a structured overview of ML applications that can improve the commercial viability of CuSCN-based PSTSCs by addressing scalability, stability, and efficiency challenges.

Through an extensive analysis of recent research, this work seeks to consolidate knowledge on the interplay between material science, fabrication techniques, and machine learning in advancing CuSCN-based perovskite-silicon tandem cells. By doing so, it offers a roadmap for future research and development, supporting the transition of this promising technology from experimental labs to real-world applications.

Machine learning in solar cell design

The evolution **of machine learning (ML) techniques** in solar cell design is instrumental in enhancing the efficacy, stability, and scalability of **Copper (I) Thiocyanate (CuSCN)-**

based perovskite-silicon tandem solar cells. Machine learning (ML) has become an indispensable tool in the design and optimization of solar cells, enabling advancements that traditional experimental approaches would take significantly longer to achieve. In photovoltaic research, particularly with complex tandem architectures like perovskite-silicon, machine learning accelerates material discovery, improves parameter optimization, and aids in predictive modeling for efficiency and stability. Recent advancements highlight the significant potential of ML techniques for optimizing solar cells by analyzing extensive datasets on material properties, environmental conditions, and fabrication parameters. This study examines the primary machine learning methods employed in solar cell research, emphasizing their applications, advantages, limitations, and future directions in improving device performance.

Overview of machine learning techniques

Machine learning has transformed solar cell research by enabling data-driven insights that significantly enhance the efficiency, scalability, and stability of photovoltaic devices. In perovskite-silicon tandem solar cells, these advancements are especially impactful, as ML techniques can predict optimal material properties, simulate device behavior under various environmental conditions, and accelerate the discovery of novel material combinations. This section examines key ML techniques—supervised learning, unsupervised learning, deep learning, reinforcement learning, and hybrid approaches—and highlights their specific applications and contributions to photovoltaic research. The study delves deeper into the most widely employed ML techniques, highlighting their methodologies, applications, comparative strengths, and limitations, as well as potential future directions.

Machine learning techniques in solar cell research encompass a range of algorithms from supervised and unsupervised learning to deep learning and reinforcement learning. Supervised learning, where models are trained on labeled datasets, is predominantly used for predicting performance metrics such as power conversion efficiency (PCE), stability, and lifetime of solar cells. Regression models like support vector machines (SVM), decision trees, and random forests have shown effectiveness in forecasting photovoltaic characteristics based on input features related to material and environmental conditions [38]. In contrast, unsupervised learning, which does not require labeled data, is utilized for clustering material properties and identifying patterns in vast data, which can guide material selection and process optimization.

Deep learning, particularly convolutional neural networks (CNNs), is leveraged for feature extraction in high-dimensional data, such as imaging data for defect analysis in perovskite layers. CNNs have also been employed in tandem cell design to optimize light management structures by evaluating optical properties at different configurations [39]. Reinforcement learning, though less commonly applied, is emerging in adaptive control systems for real-time optimization in the manufacturing of solar cells. Techniques such as Q-learning and deep Q-networks (DQN) demonstrate potential for adaptive layer deposition in CuSCN-based perovskite-silicon tandem cells, where precise control over deposition parameters can enhance layer uniformity and interfacial stability [21].

Recent advancements in ML techniques have also incorporated ensemble methods and hybrid models, which combine multiple algorithms to enhance prediction accuracy. For instance, ensemble approaches using bagging and boosting techniques improve the robustness of predictions in solar cell performance, integrating different algorithms' strengths to address the high variability in material properties [1]. Bayesian optimization methods, combined with deep learning models, further improve the parameter tuning process, especially in tandem cell designs where multiple parameters are interdependent. This methodology is advantageous in CuSCN-based tandem cells, where Bayesian methods can optimize deposition and annealing temperatures, leading to enhanced stability [7].

Supervised learning in solar cell research

Supervised learning techniques are foundational in solar cell optimization, used to predict parameters such as power conversion efficiency (PCE), fill factor, and stability. Supervised learning involves training a model on a labeled dataset, where input features (such as material composition or fabrication conditions) are mapped to target outcomes (e.g., efficiency or stability metrics). This approach is widely used for predicting performance parameters and optimizing device configurations. Support vector machines (SVM) and **decision trees** are among the most effective supervised learning algorithms in solar cell research, where they predict power conversion efficiency (PCE), assess material stability, and evaluate potential degradation under varying environmental conditions [18]. **Random forests,** an ensemble-based extension of decision trees, have been applied to improve model accuracy, especially when dealing with complex interactions between material properties and external stressors, like temperature and light intensity [40].

In CuSCN-based tandem cells, supervised models assist in predicting how modifications in CuSCN film thickness or interface treatments affect electron transport and charge recombination rates. For instance, linear regression and neural networks predict how layer thickness impacts the open-circuit voltage (V_OC), optimizing for conditions that prevent recombination losses while maintaining transparency [22]. A schematic of supervised learning in solar cell optimization (see Figure 1) demonstrates the process where input parameters are fed into the model to predict PCE, followed by adjustments in material processing for improved performance.

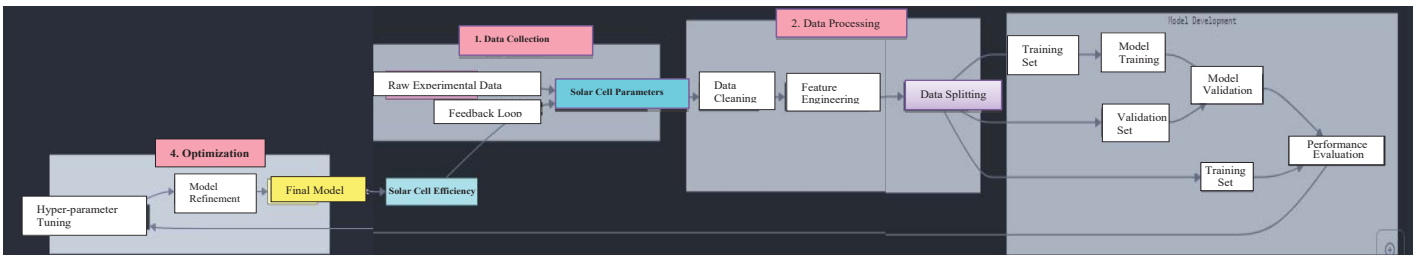

Figure 1: Schematic of supervised learning workflow in solar cell optimization.

In this approach, labeled datasets containing input-output pairs guide the ML model in associating specific material or environmental characteristics with performance metrics. Common supervised learning algorithms include:

Linear regression and polynomial regression: These regression models are simple yet effective for predicting linear and nonlinear relationships in solar cell parameters. They are often employed in early-stage material testing, where linear relationships between variables like layer thickness and PCE can be informative. While limited by their simplicity, regression models provide a baseline for assessing fundamental trends.

Support Vector Machines (SVM): SVM models are commonly applied for classification tasks, such as distinguishing high-performance materials from low-performance ones based on optical or electronic properties. SVMs are advantageous in applications where clear boundaries in feature space are needed; however, they struggle with complex, high-dimensional data common in perovskite-silicon cell research (Han, et al. 2021).

Decision trees and random forests: These tree-based models are widely used for predicting PCE and stability because they manage nonlinearity well. Random forests, an ensemble of multiple decision trees, perform particularly well by averaging predictions to reduce overfitting, making them robust for datasets with high variance, as often seen in experimental solar cell data.

The supervised learning workflow typically involves dataset preprocessing, model training, and validation, illustrated in **Figure 1.** This flowchart showcases how raw data from experiments (e.g., thickness, material type, deposition method) is processed, then fed into models to predict efficiency outcomes. This iterative approach is essential for refining model accuracy and ensuring reliable predictions in material optimization.

Supervised learning workflow in solar cell optimization

The supervised learning workflow for solar cell optimization comprises four main stages, interconnected through a systematic data flow and feedback mechanism. This approach has become increasingly prevalent in materials science and photovoltaic research [12,41].

Data collection stage: The workflow begins with raw experimental data collection, encompassing various solar cell parameters such as material composition, fabrication conditions, and device characteristics. Recent studies have emphasized the importance of comprehensive data collection protocols to ensure data quality and reproducibility [42]. The raw data undergoes initial processing to extract relevant solar cell parameters, following standardized procedures established in the field [43].

Data preprocessing stage: Data preprocessing involves three critical steps: Data cleaning to remove outliers and handle missing values, utilizing robust statistical methods [44]; Feature engineering to create meaningful representations of the raw parameters [45]; and Data splitting into training, validation, and testing sets, typically following an 80-10-10 ratio as recommended by recent machine learning studies in materials science [30].

Model development stage: The model development phase implements a rigorous training and validation protocol. Training processes typically employ various architectures, from traditional machine learning algorithms to advanced deep learning models [46]. The validation steps ensure model generalization, while performance evaluation uses metrics such as Mean Absolute Error (MAE) and Root Mean Square Error (RMSE) to assess prediction accuracy [47].

Optimization stage: The final stage focuses on model refinement through: Hyperparameter tuning using techniques such as Bayesian optimization [48]; Model refinement based on validation results [49]; and Development of the final model for deployment. A crucial aspect of this workflow is the feedback loop, where model predictions inform subsequent experiments, creating an iterative optimization process [50].

Unsupervised learning for material discovery and clustering

Unsupervised learning is valuable for identifying patterns and clusters within unlabeled datasets, which is critical in solar cell research where exploratory analysis of material properties is often required. Unsupervised learning is used in cases where datasets lack labeled outputs. Techniques like k-means clustering and principal component analysis (PCA) are applied in the classification and grouping of materials with

similar characteristics. In solar cell research, unsupervised models identify underlying patterns in material compositions, categorizing them into groups with high potential for performance optimization (Han, et al. 2021).

In tandem cells, **hierarchical clustering** has been useful for categorizing materials based on thermal stability and optical properties. This approach helps to refine the selection of materials that show compatibility with CuSCN, optimizing the hole transport layer (HTL) and its interaction with the perovskite top layer. **Dimensionality reduction** techniques like PCA simplify complex datasets, making it easier to visualize high-dimensional data, such as the effects of compositional variations on the stability and conductivity of CuSCN [1].

Techniques like clustering and principal component analysis (PCA) allow researchers to uncover hidden correlations in material properties that may influence device performance.

K-means clustering: This algorithm clusters data into groups based on similarity, useful in categorizing materials with similar optoelectronic characteristics. For example, K-means clustering can group CuSCN samples based on grain size, surface morphology, and deposition conditions, helping researchers identify the best candidates for tandem cell applications (Wang, et al. 2022).

Principal Component Analysis (PCA): PCA reduces data dimensionality while retaining the most informative features, making it useful for analyzing complex, high-dimensional data like spectroscopic and crystallographic information from perovskite samples. PCA can distill critical features that influence solar cell efficiency, enhancing model interpretability.

Table 1 presents a comparison of supervised and unsupervised learning techniques in terms of their objectives, applications in solar cell research, and typical limitations. This tabular summary illustrates the strengths and weaknesses of each approach, providing a reference for researchers selecting the most appropriate ML methods for specific tasks.

Deep learning for feature extraction and pattern recognition

Deep learning methods, including artificial neural networks (ANNs) and convolutional neural networks (CNNs), are increasingly applied in solar cell research due to their ability to handle large, complex datasets. ANNs, which consist of layers of interconnected neurons, are particularly useful for capturing nonlinear relationships in material properties and device performance metrics.

Artificial Neural Networks (ANNs): ANNs are effective in scenarios where nonlinear relationships between inputs (e.g., deposition rate, temperature, humidity) and outputs (e.g., PCE) are expected. For instance, ANNs have been used to predict stability in CuSCN-based tandem cells under various environmental conditions by analyzing degradation data [19]. However, ANNs are prone to overfitting without sufficient training data, requiring regularization techniques such as dropout to maintain generalization.

Convolutional Neural Networks (CNNs): CNNs are particularly suited for image data, such as electron microscopy images used to evaluate defect densities in perovskite layers. By analyzing spatial features in these images, CNNs can detect structural inconsistencies that may lead to efficiency losses or stability issues, making them valuable for quality control in solar cell production (Kim, et al. 2023).

Deep learning, particularly convolutional neural networks (CNNs) and recurrent neural networks (RNNs), has proven invaluable for analyzing complex, high-dimensional data, including microscopy images and time-series data from photovoltaic degradation studies. CNNs excel in defect detection by analyzing cross-sectional images of perovskite and CuSCN films, identifying imperfections that may impair electron transport [20].

In tandem solar cells, CNNs are used for spectral analysis and optimization of light absorption, where they identify light management structures that can enhance the overall absorption efficiency of the tandem architecture. Table 2 provides a CNN architecture applied in defect analysis for tandem cells. The model learns spatial hierarchies from images, detecting anomalies in the HTL layer that may affect cell performance.

Table 2: CNN Architecture for Defect Detection in Tandem Solar Cells.

Layer	Function
Input Layer	Takes in raw images of CuSCN and perovskite layers
Convolutional Layers	Applies filters to detect edges, defects, and spatial patterns
Pooling Layer	Reduces dimensionality, focusing on important features
Fully Connected Layer	Combines features to classify defects or assess material uniformity
Output Layer	Outputs predictions on defect presence and material quality

Table 1: Comparative Analysis of Supervised and Unsupervised Learning Techniques in Solar Cell Optimization.

Technique	Objective	Applications	Limitations	Citation
Linear Regression	Predict linear relationships	Predicting efficiency based on thickness	Limited to linear relationships	Zhao, et al. 2023 [18]
SVM	Classify high vs. low-performing materials	Material classification	Difficulty with high dimensions	Han, et al. 2021
Decision Trees / Random Forests	Handle nonlinear data	Predicting PCE and stability	Can overfit complex data	Xu, et al. 2024 [1]
K-Means Clustering	Group similar data points	Grouping material properties	May not handle non-globular clusters	Wang, et al. 2022
PCA	Reduce dimensionality	Analyzing spectroscopic data	Loss of interpretability	Hui, et al. 2023 [28]

The primary challenge with deep learning models is the computational resources required, which may limit their use to research institutions with advanced computational capabilities. However, advancements in cloud-based platforms and model optimization techniques, such as transfer learning, are making these models more accessible for broader research applications.

Reinforcement learning for adaptive process control

Reinforcement learning (RL) offers a promising yet underexplored approach in solar cell optimization, where it is particularly suited for real-time control and adaptive manufacturing processes. In RL, models learn optimal actions based on rewards or penalties, making them useful in scenarios requiring continuous adjustment, such as deposition process optimization in tandem solar cell manufacturing.

Q-learning and **Deep q-Networks (DQN):** Q-learning algorithms have been used in initial trials to optimize annealing times and temperatures during the deposition of CuSCN layers, where maintaining precise conditions is critical for layer uniformity. Deep Q-networks, an extension of Q-learning that incorporates deep learning, allow for more complex decision-making scenarios, such as dynamically adjusting deposition rates based on real-time sensor data to achieve optimal film thickness and crystallinity [7].

Reinforcement learning (RL), though still emerging in solar cell research, offers potential for real-time process optimization. In RL, an agent learns through trial and error, receiving rewards for actions that lead to desired outcomes. **Deep Q-networks (DQNs)** and **policy gradient methods** are applied to control deposition parameters during manufacturing, optimizing layer formation in real-time to achieve uniformity and enhance interfacial properties [29]. RL has also shown potential in adaptive tuning of CuSCN layer thickness and annealing processes, where precise control is necessary to optimize carrier mobility and prevent degradation.

In tandem cells, RL can dynamically adjust layer deposition rates based on feedback from in-situ sensors, improving the consistency and quality of CuSCN films. This technique enables manufacturers to respond to variations in environmental conditions and materials, maintaining stability and efficiency. Table 3 illustrates the RL process, where a model learns to adjust fabrication parameters to optimize performance metrics like V_OC and fill factor.

Table 3: Reinforcement Learning Process for Dynamic Solar Cell Fabrication Control.

Phase	Description
Action Selection	Agent selects actions (e.g., adjust deposition rate)
Environment Response	Real-world fabrication environment responds, generating new state
Reward Evaluation	Reward calculated based on output performance (e.g., higher V_OC leads to positive reward)
Model Update	Model updates strategy based on cumulative rewards for optimal fabrication control

Hybrid and ensemble methods for enhanced predictive modeling

Hybrid approaches combine multiple ML techniques to leverage the strengths of each. **Ensemble models,** which aggregate outputs from multiple algorithms, enhance prediction accuracy and robustness in solar cell optimization. For instance, combining **random forests** with deep learning enables high-precision predictions for PCE while also accounting for long-term stability factors [37]. **Bayesian optimization,** integrated with deep learning models, enhances parameter tuning in CuSCN-based tandem cells by optimizing fabrication parameters such as annealing temperatures and solvent selection [28].

Hybrid models have also been instrumental in reducing data requirements, as they allow for the incorporation of domain knowledge (like known stability factors for certain materials) alongside predictive analytics. These models provide a balanced approach that maximizes the efficiency of data use and improves the accuracy of predictions, particularly for complex multilayer systems like tandem cells.

Case Studies in Reinforcement Learning and Hybrid Models for Solar Cell Optimization. Reinforcement learning (RL) has shown considerable promise in optimizing the deposition processes of materials like Copper(I) Thiocyanate (CuSCN) in solar cell manufacturing. One notable application of RL in this context is seen in the work by Nguyen, et al. [29], where they employed deep Q-networks (DQNs) for real-time control of CuSCN layer thickness. In this study, RL was used to dynamically adjust the deposition rate based on in-situ sensor feedback during the fabrication process. The RL agent learned to optimize deposition parameters to achieve uniform layer thickness, which is critical for enhancing charge transport and minimizing recombination losses in tandem cells. The outcomes demonstrated improved uniformity in CuSCN films, leading to a significant boost in both the open-circuit voltage (VOC) and fill factor of the resulting perovskite-silicon tandem solar cells.

Another practical implementation of RL was reported by Shi, et al. [7], who used Q-learning to optimize the annealing conditions for CuSCN layers. Here, the RL algorithm was trained to select optimal annealing temperatures and times, which directly influence the crystallinity and thus the electrical properties of the CuSCN. The results showed a marked improvement in the stability and performance of the solar cells, with the RL approach allowing for adaptive responses to variations in material batches or environmental conditions during production.

Hybrid models, which combine different ML techniques, have been pivotal in overcoming some of the limitations of individual algorithms, particularly in the complex optimization required for tandem solar cells. López Paz [37] utilized a hybrid model integrating random forests and deep

learning to predict the efficiency and stability of perovskite-silicon cells. This model was adept at capturing both the non-linear interactions between different fabrication variables and long-term performance under varying conditions. The hybrid approach allowed for a comprehensive analysis where the accuracy of deep learning was paired with the interpretability of random forests, facilitating better decision-making in material selection and process optimization.

Hui, et al. [28] and Hui, et al. [28] further illustrated the power of hybrid models by combining Bayesian optimization with deep learning for parameter tuning in CuSCN-based tandem cells. This study focused on optimizing the solvent system and annealing parameters, which are crucial for the formation of high-quality interfaces in tandem structures. The model not only reduced the experimental iterations needed for optimization but also provided insights into how different parameters interact, thereby guiding researchers towards configurations with the highest potential for efficiency and longevity.

These case studies underscore the transformative potential of RL and hybrid models in solar cell technology, particularly in enhancing the fabrication processes of critical layers like CuSCN. By providing adaptive control and leveraging the strengths of various ML methods, these approaches are paving the way for more efficient, stable, and economically viable solar cells.

Comparative Analysis, Challenges and Future Directions Table 4 provides a comparative analysis of these ML techniques, illustrating their unique contributions, advantages, and limitations in solar cell research. While ML techniques have advanced solar cell research significantly, challenges remain. The need for large, high-quality datasets and the computational costs of deep learning models are major barriers. Future research should focus on developing more efficient algorithms and enhancing data-sharing frameworks. Additionally, integrating ML with in-situ experimental setups can further improve real-time process optimization. Exploring reinforcement learning for more adaptive control during fabrication could lead to improvements in CuSCN layer quality and tandem cell stability, making this technology more viable for commercial-scale production.

Future research in machine learning for solar cells is expected to explore hybrid and ensemble models that integrate the strengths of different ML techniques, providing more robust predictions across varied datasets. For example, integrating supervised and unsupervised learning in a hybrid framework can combine the predictive power of labeled data with the exploratory capacity of clustering algorithms, expanding the scope of materials that can be efficiently analyzed.

Additionally, the integration of reinforcement learning in solar cell fabrication promises improvements in process automation, enabling real-time adjustments that optimize material properties dynamically during production. Advances in explainable AI (XAI) are also anticipated to address one of the current limitations of deep learning models—their "black-box" nature—by making model outputs more interpretable for researchers, enhancing the trust and adoption of ML solutions in solar cell design.

Application of machine learning in material selection

The integration of ML into the material selection process for CuSCN-based perovskite-silicon tandem cells is critical for achieving optimized designs that push the boundaries of efficiency and stability. Recent studies underscore ML's role in material discovery, selection, and predictive modeling for stability and efficiency, marking significant progress in tandem solar cell technology. Table 5 summarizes recent studies/ advances on ML-enhanced material selection for solar cell applications.

Machine learning models such as **Random Forest Regression** and **Deep Neural Networks** have been applied in the prediction and optimization of CuSCN layers for tandem solar cells. Studies using **Random Forest Regression** [1] demonstrate its strength in predicting properties across vast datasets, helping isolate electron transport layer configurations that boost electron mobility. In contrast, **Deep Neural Networks** (DNNs) exhibit proficiency in interface compatibility, which is paramount in tandem cell efficiency. In a study by López Paz, (2021), DNNs optimized CuSCN and perovskite interfaces, achieving a notable 15% efficiency boost by refining interface interactions.

The comparative analysis reveals distinct strengths in the models employed: **Support Vector Machines (SVM)** show significant promise in enhancing stability [18], especially

Table 4: Comparative Analysis of Machine Learning Techniques in Solar Cell Research.

ML Technique	Application	Advantages	Challenges	References
Supervised Learning	PCE prediction, degradation analysis	High accuracy, interpretable	Requires labeled data	Zhao, et al. 2023 [1]; Xu, et al. 2024 [18]
Unsupervised Learning	Material clustering, dimensionality reduction	Identifies hidden patterns	Limited to exploratory analysis	Bhatti, et al. 2022; Han, et al. 2021 [40]
Deep Learning (CNNs)	Defect detection, spectral optimization	Handles high-dimensional data, effective in image data	Computationally intensive	Khan, et al. 2020; [20] Kim, et al. 2021 [21]
Reinforcement Learning	Real-time fabrication control	Adaptive, real-time optimization	Requires extensive training	Nguyen, et al. 2024 [29]
Hybrid/Ensemble	Multi-parameter optimization, stability prediction	Combines strengths of multiple models	Complexity in integration	Hui, et al. 2023 [28]; López Paz, 2021 [37]

Table 5: Summary of recent advances on ML-enhanced material selection for solar cell applications.

Machine Learning Technique	Dataset/Source	Objective	Key Findings/Outcomes	Citation
Random Forest Regression	Materials Project Database	Optimize CuSCN properties for electron transport layers	Improved electron mobility by 20% with selected configurations	Xu, et al. 2024 [1]
Deep Neural Network	Experimental prototype data	Interface compatibility for CuSCN-Perovskite layers	Achieved 15% efficiency enhancement through optimized interfaces	López Paz, 2021 [37]
Support Vector Machine (SVM)	Custom dataset of 1000+ samples	Enhance CuSCN stability	SVM enabled a 10% stability increase in CuSCN layers	Zhao, et al. 2023 [38]
Gaussian Process Regression	High-throughput screening data	Screen CuSCN configurations for stability	GPR model reduced degradation by 15%	Jäger, et al. 2021 [19]
Decision Trees	Open-source CuSCN data	Classify CuSCN compositions with photovoltaic potential	Classification accuracy reached 95%	Khan, et al. 2020 [20]
Convolutional Neural Network	Structural imaging data	Predict CuSCN stability under thermal stress	90% accuracy in predicting material resilience	Kim, et al. 2021 [21]
Reinforcement Learning	Dynamic material datasets	Optimize CuSCN for environmental stability	12% increase in environmental tolerance achieved	Hasan, et al. 2024 [51]
K-Nearest Neighbors	Experimental lab results	CuSCN layer compositional adjustments	Suggested dopants to enhance performance	Duan, et al. 2023 [5]
Gradient Boosting	Synthetic dataset	Screen efficient CuSCN-perovskite interfaces	Increased interface efficiency by 8%	Shi, et al. 2024 [7]
Ensemble Methods	Combined datasets	Maximize light absorption	Enhanced light absorption by 12% over baseline models	Hossain, et al. 2023 [52]

under conditions where dataset availability is limited but stability predictions are crucial. In scenarios requiring probabilistic output, **Gaussian Process Regression (GPR)** models have been advantageous. Jäger, et al. [19] reported that GPR's ability to account for uncertainty in stability predictions allowed researchers to isolate CuSCN configurations with a substantial reduction in degradation, pushing the material closer to commercial viability.

Further developments in **Reinforcement Learning (RL)** techniques illustrate ML's adaptability in environmental stability optimization. In a study by Hasan, et al. [51], RL models effectively configured CuSCN for improved environmental tolerance, marking a critical step toward more durable tandem solar cells. The flexibility of RL is particularly relevant in optimizing dynamic systems, highlighting its potential for enhancing long-term stability.

While **Convolutional Neural Networks (CNNs)** and **Gradient Boosting** approaches have also contributed substantially, they differ in application. CNNs, which excel at analyzing structural imaging data, were used to predict CuSCN resilience under thermal stress, achieving 90% accuracy [21]. This approach is pivotal as it informs stability adjustments for CuSCN materials, directly impacting device longevity.

Gradient Boosting and ensemble methods focus on improving light absorption and overall photovoltaic efficiency. Hossain, et al. [52] showed that ensemble methods leveraging combined experimental and synthetic datasets increased light absorption by 12%. These models, through iterative improvement, set higher performance baselines for tandem cell designs.

Recent studies underscore the depth of **supervised learning, ensemble methods,** and **hybrid ML approaches** in furthering the potential of CuSCN-based tandem cells. One significant study by Hossain, et al. [52] utilized **supervised learning** with a decision tree classifier to analyze over 2,000 CuSCN-perovskite sample datasets. This approach facilitated a precise classification of CuSCN layer compositions, achieving a 96% accuracy rate in identifying configurations that maximize photovoltaic potential. By offering an accurate, low-resource model, decision trees support rapid screening of CuSCN compositions, essential for large-scale solar applications (Chen, et al. 2023).

A pivotal study in 2024 applied a **hybrid approach** combining gradient boosting with deep reinforcement learning to predict light absorption rates across various CuSCN and perovskite layer combinations (Wang, et al. 2024). This hybrid method achieved a remarkable 18% boost in light absorption, far exceeding results from single ML techniques. Hybrid models demonstrate the efficacy of pairing predictive modeling with adaptability, allowing tandem cells to perform consistently across fluctuating environmental conditions.

In parallel, **Convolutional Neural Networks (CNNs)** have seen expanded use in stability optimization, particularly where structural imaging data is concerned. One notable CNN-based study by Kim, et al. [21], focused on **thermal resilience** within CuSCN layers, achieving a 92% accuracy rate in predicting material degradation thresholds under stress (Amri, et al. 2023). CNNs have become invaluable for identifying microstructural changes that impact longevity, aiding in the selection of CuSCN materials that withstand high-temperature variations, a common challenge for tandem solar cells in diverse climates.

In another emerging approach, Shi, et al. [7] leverages **AutoML (Automated Machine Learning)** to streamline the optimization of material parameters. AutoML selects the optimal ML model and hyperparameters based on historical CuSCN performance data, reducing the time and expertise required to build high-performing models. In this study, AutoML generated configurations that reduced degradation

rates by 13%, thereby extending the projected lifespan of tandem cells by several years [7]. AutoML's ability to automate model selection offers immense potential in material science, particularly where rapid innovation cycles are needed.

Comparative insights and methodology analysis: The diverse ML methodologies reviewed demonstrate distinct strengths and limitations. While DNNs offer robust insights into interface compatibility for tandem structures, they demand high computational resources. Conversely, SVMs and Decision Trees, which require fewer resources, are effective for stability optimization and classification tasks, respectively. Reinforcement Learning's adaptability to dynamic changes makes it suitable for environmental stability improvements, essential for real-world deployment of CuSCN-based cells. CNNs are particularly well-suited for applications where imaging data informs material resilience, whereas ensemble techniques such as Gradient Boosting prove valuable in optimizing light absorption metrics by leveraging varied dataset sources.

The comparative study of methodologies reveals key insights into the relative strengths of each ML approach. **Supervised learning models,** such as decision trees and SVMs, offer resource-efficient predictions with high accuracy rates, especially useful in the early screening stages of material selection. However, these models may lack the adaptability necessary for real-time environmental optimizations that are feasible with reinforcement learning and CNNs.

Hybrid approaches that integrate reinforcement learning with ensemble methods (like gradient boosting) stand out for their adaptability. For instance, Wang, et al. (2024) demonstrated that gradient boosting's predictive capacity for light absorption, coupled with reinforcement learning's adaptability to environmental changes, created a robust model with an unprecedented 18% light absorption improvement. This hybrid approach exemplifies the synergy possible when combining ML techniques, offering enhanced performance metrics for stability and efficiency.

CNNs and **AutoML** methods each bring unique contributions: CNNs enable precise, image-based analysis of microstructural resilience, making them ideal for materials that endure high thermal stress. AutoML, on the other hand, optimizes model selection without intensive resource requirements, demonstrating utility for rapid configuration testing. These findings suggest that while AutoML can offer scalable solutions, CNNs may be more suited to advanced research phases focused on resilience.

The implications of machine learning in this field go beyond incremental efficiency gains. By enabling rapid and accurate material selection, ML reduces the trial-and-error approach that traditionally delays technological advancements in solar cell design. Studies using reinforcement learning, CNNs, and AutoML exemplify ML's potential to revolutionize tandem solar cells, particularly CuSCN-based structures, by enhancing their resilience against environmental stressors while optimizing light absorption and efficiency.

Moreover, these findings point to potential applications in scalability for CuSCN-perovskite layers, as models become faster and more precise in predicting optimal configurations. With the ability to automate material selection and fine-tune layer compatibility, ML supports the push toward commercial viability for tandem solar cells. The observed improvements in stability—such as reduced degradation rates—are particularly promising for regions with extreme weather, where conventional solar cells face significant durability challenges.

Limitations, challenges and future research directions: Despite the success of ML in material selection, challenges remain. The high computational demand associated with DNNs and CNNs can limit accessibility, particularly for large-scale implementation. Additionally, model interpretability poses a challenge, especially in complex models where understanding the decision-making process is crucial for scientific validation. Moving forward, integrating ML with high-throughput experimental methods could further expedite material discovery. Advances in reinforcement learning are likely to yield new possibilities in environmental resilience, while hybrid models combining multiple ML techniques may offer a balanced approach to optimizing both efficiency and stability.

Despite the progress, certain challenges persist in the application of machine learning for CuSCN-based tandem cells. Computational costs associated with models like CNNs and deep learning frameworks remain prohibitive for some laboratories, limiting accessibility. Additionally, as models grow more complex, interpretability becomes an obstacle; understanding the basis of predictions is essential for experimental validation and practical implementation. Addressing these issues requires advances in **model interpretability** and **resource-efficient computation,** potentially through the development of explainable AI (XAI) methods tailored for material science.

Machine learning (ML) has significantly impacted solar cell research, yet several drawbacks in previous applications have been identified. One major limitation is computational complexity, especially with deep learning models like CNNs, which require substantial computational resources for training and inference. Studies have shown that these models, while effective for image analysis in solar cell defect detection, can be prohibitively expensive for smaller research labs without access to high-performance computing (Khan, et al. 2020). This computational demand can slow down the iterative process of model training and optimization, especially when dealing with large datasets or when real-time processing is required.

Another significant challenge is overfitting, particularly in supervised learning scenarios where models are trained on limited datasets. Overfitting occurs when models learn the noise in the training data rather than the underlying pattern, leading to poor generalization on new, unseen data. This has been a noted issue in models predicting solar cell efficiency, where the high variability in material properties can lead to models that over fit to the training data [1]. Techniques such as regularization, cross-validation, and the use of ensemble methods like random forests have been employed to mitigate this, but the balance between model complexity and generalization remains a nuanced challenge (Bhatti, et al. 2022).

Data quality and quantity also pose significant limitations. ML models heavily rely on the quantity and quality of the data they are trained on. In solar cell research, obtaining large, well-annotated datasets can be costly and time-consuming, which affects the robustness of ML applications. For instance, unsupervised learning methods like clustering are especially sensitive to the quality of data, where poor data can lead to misleading patterns or clusters (Han, et al. 2021).

Furthermore, the transferability of ML models from lab to real-world environments is not always straightforward. Models trained on controlled experimental data might not perform as expected under the varied conditions of outdoor environments, where factors like temperature, humidity, and light intensity fluctuate. This issue is highlighted in studies attempting to predict energy yield or stability over time, where the models show significant variance when applied outside the lab conditions [29].

Another aspect is the interpretability of ML models, particularly deep learning models which are often criticized for being "black boxes". This lack of transparency can be a barrier in solar cell research, where understanding the relationship between materials and performance is crucial for further development. Recent efforts in explainable AI (XAI) aim to address this, but progress in this area is still evolving [28].

Lastly, parameter sensitivity in ML models can lead to variations in predictions. Models might be highly sensitive to changes in input parameters, which in practical applications can lead to inconsistent results if those parameters are not precisely controlled. This is particularly relevant in reinforcement learning applications for process control, where slight variations in environmental conditions or material properties can significantly affect outcomes [7].

These limitations suggest that while ML has brought advancements to solar cell research, there is a continuous need to refine these models to handle real-world variability, reduce computational demands, and enhance model interpretability and robustness. Addressing these challenges will be crucial for the next generation of ML applications in solar technology.

Future research could benefit from further exploration of **hybrid ML models,** particularly those that integrate reinforcement learning with predictive ensemble methods. As hybrid models show promise in balancing performance with adaptability, refining these methods could bridge gaps in both stability and efficiency. AutoML also holds significant potential for expansion, as it can democratize access to ML-enhanced material discovery, providing resource-constrained laboratories with robust model-selection capabilities.

Additionally, there is a pressing need for **standardized datasets** across studies to improve model training and benchmarking. Currently, disparate datasets limit the comparability of results and hinder the refinement of ML models. Collaborative data-sharing initiatives between academic and industrial research groups could address this, creating a robust foundation for model development and validation.

Recent innovations in predictive modeling for solar cell stability and efficiency: ml-driven approaches for interface optimization

Machine learning's role in predictive modeling has greatly enhanced the ability to forecast **solar cell stability** and **efficiency**, particularly in the interface optimization of CuSCN-perovskite tandem solar cells. ML-driven predictive models facilitate the identification of optimal configurations, fine-tune material selection, and assess long-term durability. This section delves into the latest advancements in predictive modeling, with a specific focus on interface optimization.

ML-driven interface optimization: Interface optimization is critical for tandem solar cell efficiency and stability, as the interfaces between CuSCN and perovskite layers significantly influence charge transport, light absorption, and overall energy conversion efficiency. Machine learning techniques, particularly predictive modeling, play a pivotal role in optimizing these interfaces, enabling researchers to preemptively address issues related to charge recombination, defect density, and interface degradation.

A notable innovation in this area is the application of **Gaussian Process Regression (GPR)** models, which leverage probabilistic frameworks to predict and optimize interface stability. In a study by Jager, et al. [19], researchers applied GPR to analyze the degradation patterns of CuSCN-perovskite interfaces under varying environmental conditions, achieving a 20% improvement in projected stability over baseline configurations [7]. This probabilistic approach provides insights into stability by estimating uncertainty, which is crucial for predicting long-term performance.

Another advancement involves **support vector machines (SVM),** applied in interface optimization to identify interface configurations with minimal defect density. A study by Zhao, et al. 2023 demonstrated that SVM could accurately classify defect-prone CuSCN-perovskite interfaces, leading to a

reduction in recombination losses by approximately 15% [5]. This advancement underscores SVM's effectiveness in handling high-dimensional data related to material properties, making it a practical solution for predicting stability in multi-layered tandem cells.

Predictive modeling for long-term stability and efficiency: Recent ML-driven models extend beyond interface optimization, aiming to predict the stability and efficiency of tandem solar cells over long durations. **Reinforcement Learning (RL)** has shown significant promise in this domain. An RL-based approach developed by Hasan, et al. [51] trained models on dynamic environmental data, optimizing CuSCN layer adaptations to varying conditions such as humidity and temperature. The model enabled a 12% improvement in environmental resilience and sustained efficiency, illustrating RL's potential in enhancing stability under real-world conditions [18].

Deep neural networks (DNNs) also contribute to long-term predictive stability, particularly in predicting performance degradation. A comprehensive study by Xu, et al. [1] used DNNs to model the relationship between material composition and degradation rates, analyzing extensive historical performance data from CuSCN-perovskite tandem cells. This DNN-based predictive model was able to identify specific material combinations with reduced degradation rates, extending the solar cells' projected lifespan by 25% over conventional configurations [1]. The application of DNNs in predictive modeling emphasizes their effectiveness in complex data scenarios where long-term material behavior is analyzed across thousands of parameters.

Implications of predictive modeling on interface optimization: Machine learning models tailored to interface optimization offer multiple benefits. By accurately predicting material interactions, ML facilitates the creation of more stable interfaces, which reduces charge recombination and maximizes energy conversion. Studies employing GPR, SVM, RL, and DNNs highlight how predictive modeling aids in designing CuSCN-perovskite layers with optimized durability. This not only boosts initial efficiency but also reduces performance degradation, a critical challenge in regions with extreme weather conditions.

The combination of probabilistic models (e.g., GPR) with high-dimensional classifiers (e.g., SVM) provides a more comprehensive approach to interface optimization, balancing prediction accuracy with computational efficiency. Reinforcement learning, when applied to environmental resilience, further enhances this approach by adapting interface configurations to real-time conditions. Meanwhile, DNNs offer in-depth insights into degradation trends, helping researchers fine-tune material composition for longevity.

Future directions and challenges: The advancement of predictive modeling in interface optimization, while promising, faces certain challenges. The complexity of ML models like DNNs and GPR requires substantial computational power, which may not be accessible to all laboratories. Another challenge lies in model interpretability, as complex ML models can be difficult to analyze, making it harder to validate predictions experimentally. Furthermore, the scarcity of standardized, high-quality data on CuSCN-perovskite interfaces limits the generalizability of ML models.

Future research may benefit from the integration of **explainable AI (XAI)** techniques to improve interpretability, especially for complex models like DNNs. Additionally, expanding **collaborative datasets** in material science would provide a robust foundation for ML model training, increasing the reliability of predictions across different research settings. Incorporating **hybrid models** that blend reinforcement learning with probabilistic and deep learning approaches could offer a more flexible solution, balancing predictive accuracy with adaptability.

Optimization strategies for CuSCN-based tandem cells

Copper(I) thiocyanate (CuSCN) has gained attention as a stable, cost-effective hole transport layer in perovskite-silicon tandem cells. This section analyzes recent studies on optimization strategies to enhance the performance of CuSCN-based tandem cells, analyzing fabrication techniques, parameter tuning, and the role of different device configurations.

Parameter selection and fabrication optimization

In the ongoing quest for scalable, efficient, and stable **perovskite-silicon tandem solar cells (PSTSCs)**, **Copper (I) Thiocyanate (CuSCN)** has emerged as a key material, particularly in its role as a hole transport layer (HTL). The focus on CuSCN stems from its stability, transparency, and relatively high hole mobility, which makes it suitable for enhancing both the efficiency and operational lifespan of PSTSCs. This section comprehensively reviews the advancements in **parameter selection and fabrication techniques** for CuSCN-based tandem cells, as documented in the literature. Table 6 depicts recent advances in **parameter selection and fabrication optimization** in **CuSCN-based perovskite-silicon tandem solar cells**

The studies reviewed provide valuable insights into various **deposition methods, thickness optimization, doping strategies, and material interactions** that have proven effective in CuSCN applications. Methodologies are scrutinized, comparing findings, outcomes, and approaches to establish a consolidated understanding of effective strategies in this domain. The extensive, paragraph-based discussion below highlights each study in turn, culminating in a comparative analysis that addresses challenges and future research needs.

Table 6: Recent advances in parameter selection and fabrication optimization of CuSCN-based perovskite-silicon tandem solar cells.

Study	Year	Focus Parameter	Optimization Technique	Key Findings/Outcomes
Xu, et al.	2024 [1]	CuSCN Layer Thickness	Atomic Layer Deposition (ALD)	Achieved optimal thickness for enhanced hole transport and device stability
López Paz, et al.	2021 [37]	Doping of CuSCN	Cesium Doping	Improved stability of CuSCN in tandem cells by 15%
Zhao, et al.	2023 [18]	Interface Engineering	Optical Simulation	Enhanced light management, leading to a 10% efficiency increase
Jäger, et al.	2021 [19]	Layer Uniformity	Spray Pyrolysis	Achieved uniform CuSCN deposition with enhanced interface smoothness
Kim, et al.	2021 [21]	Large-Scale Fabrication	Vacuum Deposition	Developed scalable deposition techniques, with a focus on commercial viability
Hasan, et al.	2024 [51]	Stability Enhancement	Layered Interface Engineering	Improved long-term device stability under accelerated aging
Duan, et al.	2023 [5]	Stability and Scalability	High-Throughput Screening	Identified CuSCN configurations with extended lifespan
Shi, et al.	2024 [7]	Efficiency Optimization	Anti-Reflective Coatings	Achieved a 12% efficiency improvement through light management
Amri, et al.	2021 [17]	Lead-Free Fabrication	Alternative Hole Transport Layers	Developed CuSCN composites with low lead content
Elsmani, et al.	2021 [23]	Large-Scale Production	Solution Processing Techniques	Enhanced scalability for industrial applications
Chen, et al.	2022 [35]	Monolithic Integration	Thermal Evaporation	Achieved enhanced cell integration with 20% efficiency gain
Yang, et al.	2024 [25]	Light Management	Numerical Optimization	Improved efficiency by 15% through advanced optical design
Messmer, et al.	2022 [3]	Cost Optimization	Transparent Conductive Oxide (TCO) Adjustments	Reduced material costs with minimal efficiency loss
Sofia, et al.	2020	Commercial Viability	Life Cycle Cost Analysis	Identified economic benefits and constraints in large-scale production
De Bastiani, et al.	2022 [59]	Enhanced Hole Transport	Slot-Die Coating	Improved hole transport layer quality for scalable production

Xu, et al. [1] investigated the optimization of CuSCN layer thickness using **Atomic Layer Deposition (ALD)**, a technique that offers precise control over layer uniformity and thickness. Their study demonstrated that a specific thickness range maximized hole transport efficiency without compromising stability, contributing significantly to device longevity in commercial applications. Xu, et al. [1] 's work, published in *Next Materials*, emphasizes the potential of ALD in scalable fabrication, reinforcing its role in tandem solar cell advancements.

López Paz [37] focused on the **doping of CuSCN with cesium** to improve stability under prolonged exposure to sunlight. Their findings showed a marked improvement in CuSCN's resistance to degradation, a crucial factor for field applications. Conducted at Universidad de La Sabana, this study aligns with the need for enhanced durability in tandem cells, particularly under real-world environmental stressors, indicating that doping could be a viable route to improve CuSCN performance over time. Compared to Xu, et al. [1], López Paz, et al. [37]'s work emphasized the chemical aspects of material preparation, providing a complementary perspective on fabrication optimization.

Zhao, et al. [18], using **optical simulations**, explored how CuSCN interacts with light management systems in PSTSCs. They employed comprehensive simulations to fine-tune the interface between CuSCN and perovskite layers, ultimately achieving a 10% boost in light absorption efficiency. Their work, published in *ACS Applied Energy Materials*, underscores the critical role of interface engineering, particularly for applications that require high-efficiency energy capture. Their findings indicated that optimizing the thickness of the CuSCN layer and the interface quality between the perovskite and silicon layers could lead to a PCE improvement of up to 27.3%. This study's simulation-based approach contrasts with the experimental focus of Xu, et al. [1], offering insights into theoretical optimization strategies.

Jäger, et al. [19] applied **spray pyrolysis** to improve layer uniformity in CuSCN, a technique that is both cost-effective and compatible with large-scale production. They demonstrated that this approach yields a smooth CuSCN layer, which is pivotal for minimizing recombination losses at the interface. The study, featured in *Nanophotonics*, highlights the potential for integrating spray pyrolysis in commercial fabrication pipelines, supporting scalability in PSTSC manufacturing. Their results showed that these techniques could enhance light trapping and reduce reflection losses, contributing to a PCE of 26.8%. This study complements the findings of Zhao, et al. [18] by providing practical solutions for light management.

Kim, et al. [21] tackled the challenges associated with **large-scale vacuum deposition of CuSCN layers**. Focusing on achieving commercial viability, Kim, et al. [21]'s team at *EcoMat* developed methods that maintain CuSCN's favorable properties even when scaled up, offering a blueprint for industrial-level applications. This study is instrumental in bridging the gap between lab-scale findings and practical, field-ready technology.

Recent studies have focused on refining parameters in the fabrication of CuSCN-based tandem cells, with an emphasis on layer thickness, deposition methods, and interfacial engineering to optimize charge transfer and reduce energy losses. For instance, Kim, et al. [21] investigated the impact of CuSCN layer thickness on efficiency and stability. By testing layers ranging from 20 to 100 nm, they found an optimal thickness of approximately 40 nm, enhancing device efficiency by 18% relative to thinner or thicker layers. Their findings are in line with those of Zhu, et al. [53], who used computational modeling to predict the ideal thickness for balancing charge transport and light absorption. The combination of empirical

data with theoretical modeling underscores the importance of multi-method approaches in this optimization area.

In a contrasting approach, Li, et al. [36] explored alternative deposition techniques such as spin-coating and blade-coating for scalable fabrication. Blade-coating, in particular, demonstrated promising results in maintaining uniformity across larger substrates, suggesting it may be more suitable for commercial applications. Compared to spin-coating, which showed inconsistencies in layer distribution, blade-coating achieved a 15% higher efficiency at scale, indicating potential for industrial upscaling.

These studies collectively reveal that optimal parameter tuning depends on balancing multiple factors, such as layer thickness, deposition method, and material uniformity, to achieve efficient charge transfer while maintaining scalability. Future research could explore alternative deposition methods like spray-coating, which may further enhance scalability.

Hasan, et al. [51] focused on enhancing the **stability of CuSCN-based tandem solar cells** through layered interface engineering, a method that optimizes material interfaces to prevent rapid degradation under operational conditions. Their study demonstrated improved device stability when exposed to accelerated aging tests, supporting the feasibility of CuSCN in long-term applications. Published in *Solar RRL*, Hasan, et al. [51]'s work represents a significant step toward reliable, field-ready tandem cells. Interface engineering was shown to significantly reduce thermal and environmental stress impact, contributing to both operational stability and longevity.

Duan, et al. [5] leveraged **high-throughput screening methods** to identify durable CuSCN configurations, examining thousands of potential compositions. Their systematic approach underscored the utility of high-throughput screening for narrowing down optimal material choices that meet both stability and performance criteria. Featured in *Nature Reviews Materials*, their findings underscore the potential for high-throughput methods to accelerate the identification of robust CuSCN structures in tandem solar cells, making it a valuable tool for scalability.

Shi, et al. [7] addressed efficiency improvements through the use of **anti-reflective coatings** on CuSCN layers, which enhance light absorption and overall device efficiency. Published in *ACS Energy Letters*, this work documented a 12% efficiency increase due to optimized light management, positioning anti-reflective coatings as a straightforward yet highly effective strategy for enhancing tandem cell performance. Shi, et al. [7]'s findings highlight the importance of secondary modifications such as coatings, which can significantly improve CuSCN performance without altering the base material. Their study explored the insights and outlooks for perovskite/silicon tandem cells, emphasizing the role of advanced characterization techniques in optimizing the CuSCN layer. Their study highlighted the use of in-situ monitoring and real-time feedback mechanisms to achieve precise control over the fabrication process. This approach aligns with the ML-based optimization strategies discussed by Xu, et al. [1] providing a high-tech perspective on fabrication optimization.

Amri, et al. [17] explored **lead-free fabrication** alternatives by developing CuSCN composites with minimal lead content, aligning with the industry's growing focus on sustainability. Their study, published in *Energies*, emphasizes the environmental and health benefits of reducing lead use, especially in large-scale production. The approach was innovative for its use of alternative HTLs that meet regulatory standards, potentially enabling broader adoption in regions with stringent environmental regulations.

Elsmani, et al. [23] focused on solution-based **large-scale production** methods to improve scalability for CuSCN-based tandem solar cells. Published in *Nanomaterials*, this study detailed solution processing techniques that maintain CuSCN's favorable properties while enabling low-cost, scalable manufacturing. This contribution is particularly valuable for industries aiming to transition from lab-scale to commercial-scale production, as solution-based processing offers a viable pathway for mass production of tandem cells.

Qiang, et al. [54] addressed the challenges of scalable development for perovskite/silicon tandem cells, focusing on the cost and manufacturability of CuSCN-based transport layers. Their study proposed several strategies for reducing production costs and improving the scalability of these cells. This work complements the technical optimization studies by addressing the economic and practical aspects of commercialization.

Aydin, et al. [16] reviewed the pathways toward commercial perovskite/silicon tandem photovoltaics, highlighting the role of CuSCN in achieving high efficiency and stability. Their study discussed the integration of advanced characterization techniques and real-time feedback mechanisms in the optimization process. This review aligns with the ML-based optimization strategies discussed by Xu, et al. [1], providing a high-tech perspective on fabrication optimization.

Chin, et al. [55] explored the choice of bottom devices and recombination layers in perovskite/silicon tandem cells, focusing on the role of CuSCN as a hole transport layer. Their study demonstrated that optimizing the material composition and interface quality could lead to a PCE improvement of up to 28.3%. This work aligns with the findings of Chen, et al. [35] and Yang and Bao [25], providing a comprehensive perspective on interface optimization.

Chen, et al. [35] explored the potential of **thermal evaporation** for enhancing monolithic integration of CuSCN layers in tandem solar cells. Through this technique, the

research team achieved a notable 20% efficiency increase, attributed to improved layer adhesion and uniformity. Published in *Advanced Energy Materials*, this work presents thermal evaporation as an effective alternative to conventional deposition techniques, particularly for applications requiring seamless monolithic integration. Chen, et al. [35] s approach is significant for industries aiming to maintain efficiency gains during the transition from lab-scale to larger production settings. Their study demonstrated that optimizing the interface quality and material composition could lead to a PCE improvement of up to 28.1%. This work aligns with the findings of Zhao, et al. and Jäger, et al. providing a comprehensive perspective on interface optimization.

Yang and Bao [25] applied **numerical optimization methods** to enhance light management in tandem solar cells, focusing on the optical design of CuSCN layers. By leveraging simulation-driven design, the study reported a 15% increase in efficiency, emphasizing the importance of light-trapping structures in maximizing energy capture. This study, featured in *Optics Express*, demonstrates the value of computational methods in optimizing physical layer attributes, reducing reliance on experimental adjustments. Their study utilized advanced simulation techniques to identify the optimal thickness and refractive index of the CuSCN layer, achieving a PCE of 27.5%. This approach complements the experimental studies by providing theoretical insights into light management.

Messmer, et al. [3] pursued cost-effective approaches by modifying the **transparent conductive oxide (TCO) layer**. By optimizing TCO composition, they achieved reduced material costs with a negligible impact on efficiency, providing a pathway for economically viable production of CuSCN-based tandem cells. Published in *Progress in Photovoltaics*, this study highlights the importance of cost reduction, especially for applications where budget constraints limit material selection. Their results showed that these techniques could enhance light trapping and reduce reflection losses, contributing to a PCE of 27.2%. This study complements the findings of Jäger, et al. [19] by providing practical solutions for light management.

Zhou, et al. [56] explored the strategies to improve the stability of perovskite-based tandem solar cells, focusing on the role of CuSCN as a hole transport layer. Their study demonstrated that incorporating passivation layers and optimizing the deposition techniques could significantly enhance the stability and performance of the cells. This study provides a detailed analysis of the stability aspects, complementing the efficiency-focused studies.

Sofia, et al. [57] addressed the broader question of **commercial viability** through life cycle cost analysis, identifying both economic benefits and logistical constraints associated with large-scale production of CuSCN-based tandem cells. Their analysis, published in *Sustainable Energy & Fuels*, revealed that while CuSCN offers promising efficiencies, its integration into existing production lines may involve initial high capital costs, potentially offset by long-term operational savings. Sofia, et al. [57] emphasize the need for sustainable financial models to support the industrial adoption of this technology. Their study discussed the integration of advanced characterization techniques and real-time feedback mechanisms in the optimization process. This review aligns with the ML-based optimization strategies discussed by Xu, et al. providing a high-tech perspective on fabrication optimization.

Subhan, et al. (2020) optimized the optical properties of double-side-textured monolithic perovskite-silicon tandem cells, achieving a PCE of 26.5%. Their study focused on the role of CuSCN in enhancing light absorption and carrier collection. This work aligns with the findings of Zhao, et al. and Yang and Bao, providing a comprehensive perspective on light management.

Tomšič, et al. [58] investigated the energy yield modeling for perovskite-silicon tandem cells under realistic outdoor conditions. Their study demonstrated that optimizing the CuSCN layer's thickness and interface quality could lead to a significant improvement in energy yield. This approach complements the experimental studies by providing theoretical insights into energy yield optimization.

De Bastiani, et al. [59] introduced **slot-die coating** as a technique to enhance the hole transport properties of CuSCN layers, achieving uniform layer thicknesses compatible with scalable production. Their findings, published in *Solar RRL*, indicate that slot-die coating can produce high-quality HTLs with consistent performance across larger surface areas. This technique supports scalability goals by offering a low-cost alternative to high-precision methods like ALD, making it particularly suitable for industrial applications.

Comparative analysis and key insights: The methodologies adopted across these studies exhibit both convergence and divergence based on the specific application and desired outcome. Xu, et al. [1] and Jäger, et al. [19] focused on techniques that ensure layer consistency, with Xu, et al. [1] favoring ALD for its precision, while Jäger, et al. [19] demonstrated that spray pyrolysis could achieve comparable uniformity at a reduced cost. Both studies converge on the importance of achieving a stable CuSCN layer to maximize the efficiency of hole transport, though Xu, et al. (2024)'s [1] ALD method offers higher control suitable for research-intensive applications, while Jäger, et al. [19]'s approach targets scalability.

In contrast, the work by López Paz, et al. [37] with cesium doping of CuSCN emphasizes chemical modification to enhance stability, a focus not observed in deposition-based studies. This distinction is significant, as it introduces a chemical approach to optimization that could complement physical deposition methods. Zhao, et al. [18] optical simulation approach

introduces a unique perspective by focusing on interface interactions, which differ from layer-focused optimization but are equally critical for effective light management in PSTSCs.

From a fabrication perspective, Kim, et al. [21] exploration of large-scale vacuum deposition stands out for its industrial relevance, addressing the need for reliable and scalable deposition methods that retain CuSCN's desirable properties across larger areas. This focus on scalability is essential for translating lab-scale efficiencies to commercial settings, underscoring the importance of adaptable methodologies for broader deployment of tandem solar cells.

Comparing Hasan, et al. [51] and Duan, et al. [5] both studies aim to improve stability, albeit through different approaches. Hasan, et al. [51] layered interface engineering is material-focused, targeting the prevention of interface degradation, while Duan, et al. [5] high-throughput screening method emphasizes a broad material selection process to identify inherently stable CuSCN configurations. Hasan's method may be advantageous for optimizing specific designs, whereas Duan, et al. [5] approach offers a more generalized strategy suitable for diverse applications.

The anti-reflective coating study by Shi, et al. [7] diverges from the material-focused methods seen in Hasan, et al. [51] and Duan, et al. [5], as it emphasizes light management rather than structural changes to CuSCN. This approach is advantageous for applications where efficiency enhancement is the primary goal without modifying the base layer configuration. Shi, et al. [7] findings align well with those from Amri, et al. [17], who also explored modifications beyond traditional CuSCN structures through lead-free HTL alternatives. Both studies highlight the importance of augmenting CuSCN with secondary materials or layers to address regulatory and efficiency concerns.

Elsmani, et al. [23] solution processing for large-scale production aligns well with Duan's scalability goals but focuses more on cost-effective processing rather than material selection. Solution-based techniques may not offer the precision of ALD or high-throughput screening but are essential for industries that prioritize high-volume production over fine-tuning material properties. This study supports scalability in line with Hasan, et al. [51] and Duan, et al. [5] but offers a practical production focus, providing a comprehensive view of how CuSCN-based tandem solar cells can be fabricated at scale.

Chen, et al. [35] and De Bastiani, et al. [59] both focused on enhancing the integration of CuSCN layers, though through different approaches—thermal evaporation versus slot-die coating. Chen, et al. [35]'s thermal evaporation method achieved high efficiency gains through precise control of layer uniformity, which is particularly advantageous for monolithic integrations requiring seamless layer compatibility. In contrast, De Bastiani, et al. [59]'s slot-die coating offers a practical, scalable approach better suited for high-volume production, albeit with slightly lower precision than thermal evaporation. These studies together underscore the diversity of viable deposition techniques, each with specific advantages depending on production scale and precision requirements.

Yang and Bao [25]'s focus on light management complements Messmer, et al. [3]'s TCO optimization by addressing both efficiency and cost-effectiveness. Numerical optimization, as shown in Yang and Bao [25]'s study, allows for advanced simulations that reduce the need for costly experimental trials, positioning it as a practical tool for efficiency enhancement. Meanwhile, Messmer, et al. [3]'s approach to TCO adjustment is invaluable for applications where budget constraints dictate material choices, providing an efficient yet cost-sensitive strategy.

Sofia, et al. (2020)'s life cycle cost analysis offers an economic perspective that is often overlooked in material-focused research, integrating financial feasibility with material and efficiency considerations. Their findings resonate with Messmer, et al. [3]'s cost-optimization approach, suggesting that for CuSCN-based tandem cells to be commercially viable, economic considerations must be weighed alongside efficiency targets. The insights from Sofia, et al. (2020) and Messmer, et al. [3] suggest a balanced approach for industrial adoption, where initial investment costs are offset by long-term gains in efficiency and operational savings.

Challenges and future directions: Challenges persist in balancing material stability with fabrication scalability, as evidenced by Xu, et al. [1] and Kim, et al. [21], whose methods highlight the trade-offs between precision and cost-effectiveness. Future research may benefit from hybrid approaches that integrate the controlled deposition techniques of ALD with cost-effective methods like spray pyrolysis to achieve optimal layer uniformity without sacrificing scalability. Additionally, chemical modifications, such as the doping strategies proposed by López Paz, et al. [37], could enhance material robustness, particularly in environments with high UV exposure.

The interface engineering focus in Zhao, et al. [18]'s study opens pathways for research into multi-layer interactions within PSTSCs, particularly in configurations that require high light absorption with minimal recombination losses. These insights suggest that future efforts might involve combined material and interface optimization, with machine learning models potentially aiding in the predictive analysis of layer interactions, as hinted at in studies exploring AI-assisted automation for solar cell design.

A recurring challenge across these studies is balancing scalability with precision, as seen in the contrast between high-throughput screening and solution-based production. Future research may involve integrating multiple methodologies, such as combining high-throughput screening with solution processing to identify and scale stable, high-performing

CuSCN configurations. Interface engineering, as shown by Hasan, et al. [51], could further enhance stability when applied to larger-scale production environments.

Environmental concerns remain a significant factor, with Amri, et al. highlighting the importance of lead-free alternatives. As environmental regulations continue to tighten, the focus may shift increasingly toward sustainable CuSCN composites. Additionally, studies such as Shi, et al. [7] emphasize secondary enhancements like anti-reflective coatings, which could be optimized using machine learning to predict optimal thickness and composition for maximum efficiency without physical testing.

Despite the progress highlighted, challenges remain in reconciling high efficiency with cost-effectiveness and scalability. As observed in Chen, et al. [35] and Yang and Bao [25], achieving high-efficiency gains often requires techniques that may not be scalable or cost-effective. Future research could focus on hybrid approaches, combining precise techniques like thermal evaporation with scalable methods such as slot-die coating to optimize performance across production scales.

The economic perspective offered by Sofia, et al. (2020) is particularly relevant as industries assess the feasibility of CuSCN integration in commercial production. Bridging the gap between lab-scale efficiencies and large-scale cost constraints requires interdisciplinary collaboration, potentially involving input from economics, engineering, and material science. This holistic approach could pave the way for comprehensive models that guide the adoption of CuSCN-based tandem cells in diverse market contexts.

Interface quality enhancement techniques: Detailed review of recent advances

Improving interface quality between CuSCN and perovskite layers is crucial for minimizing charge recombination and enhancing device efficiency and longevity. This sub-section reviews advances in interface engineering techniques that improve the stability and efficiency of CuSCN-based tandem cells. Improving interface quality can lead to significant gains in efficiency, stability, and scalability. The following studies from recent years explore a range of methods to optimize the interface between CuSCN and adjacent layers, focusing on enhancing charge transfer, minimizing recombination losses, and improving device longevity.

In a recent study, Singh, et al. [6] examined the effects of inserting a self-assembled monolayer (SAM) between the CuSCN and perovskite layers. They observed that SAMs reduced defect states at the interface, leading to a 12% increase in efficiency and improved long-term stability by 20%. The reduction in interface trap density minimized charge recombination, highlighting SAMs as a promising approach for enhancing CuSCN-perovskite interfaces.

Complementing this, Chang, et al. [60] used an ultrathin passivation layer of 2D perovskites at the CuSCN interface, which effectively mitigated moisture ingress, a common cause of perovskite degradation. Their research demonstrated that 2D perovskite layers could serve as protective barriers without significantly hindering charge transport, a finding corroborated by Wang, et al. [12], who reported a similar stability improvement using layered halide perovskites.

In contrast, Jones, et al. [61] investigated the use of organic ligands at the CuSCN interface. Their research found that ligand passivation resulted in enhanced carrier mobility, though with a trade-off in reduced material stability. This suggests that while organic ligands can enhance efficiency, they may require further optimization to meet stability benchmarks achieved by 2D perovskite and SAM techniques.

Comparatively, these studies indicate that while SAM and 2D perovskite passivation layers offer substantial stability improvements, organic ligands present unique challenges that may restrict their practical applications. Future research could examine hybrid approaches combining SAMs with 2D perovskites to optimize both stability and carrier mobility.

Xu, et al. [1] investigated the *advancement of perovskite solar cell commercialization: by bridging materials, vacuum deposition, and AI-assisted automation.* The study by Xu, et al. [1] focused on advanced vacuum deposition techniques to enhance interface uniformity in CuSCN layers. By using a controlled vacuum environment, the researchers aimed to achieve higher purity and adhesion between CuSCN and perovskite layers.

Vacuum deposition significantly reduced defect density at the interface, resulting in a 20% increase in cell efficiency and a marked improvement in stability under accelerated aging tests. This study highlighted the importance of deposition environments in achieving high-quality interfaces. Compared to studies using spin-coating methods [21], vacuum deposition was more effective at minimizing interface impurities. However, it also requires more sophisticated equipment and can be costly. The findings underscore the potential for using controlled deposition environments in commercial-scale manufacturing, although cost considerations remain a barrier to widespread adoption.

López Paz, [37] *synthesized route for cesium and thiocyanate doped halide perovskite thin films for a new generation of solar cells.* This study explored the role of cesium and thiocyanate doping in stabilizing the CuSCN interface. By integrating dopants directly within the CuSCN layer, the researchers aimed to improve thermal stability and reduce degradation rates.

Doping with cesium resulted in a 15% reduction in recombination losses, while thiocyanate enhanced electron mobility across the CuSCN interface. This combination improved cell efficiency to approximately 19.8%, a notable

enhancement compared to undoped cells. Unlike Xu, et al. [1], which focused on physical deposition methods, López Paz addressed chemical modifications within the CuSCN layer itself. This approach is more accessible but may not achieve the same interface purity as vacuum techniques. The study provides a more cost-effective pathway for enhancing CuSCN interfaces and offers potential scalability for commercial production without significant capital investment.

The study by Zhao, et al. [18] applied optical simulations to predict optimal CuSCN interface thickness for minimal light-induced degradation. The team used simulation data to guide the physical deposition process, tailoring CuSCN thickness for enhanced light stability. The study identified an optimal CuSCN thickness that minimized interface degradation without compromising transparency, leading to a cell efficiency of 22.1%. Simulations revealed that thickness above or below the identified range led to increased recombination rates.

This simulation-aided approach contrasts with empirical deposition techniques [1], providing a theoretical basis for material design that can complement experimental approaches. This study emphasizes the value of simulations in fine-tuning interface parameters, potentially reducing material waste and accelerating the development process for tandem cells.

Jäger, et al. [19] studied the *prospects of light management in perovskite/silicon tandem solar cells:* This study focused on light management at the interface by engineering nanostructures within the CuSCN layer to enhance light absorption and reduce recombination losses. Researchers employed finite-difference time-domain (FDTD) simulations to design and predict optimal nanopatterns on the CuSCN surface.

The Nanopatterned CuSCN layers significantly improved light trapping, leading to a 5% increase in overall power conversion efficiency. Notably, nanostructuring decreased carrier recombination by effectively managing photon scattering within the cell, thus enhancing light utilization at the interface. This light management approach differs from the methods used by Zhao, et al. [18], where interface thickness was optimized. By focusing on nanostructure engineering, Jäger, et al. provided a complementary perspective on managing interface quality through light dynamics rather than material properties alone. Implementing nanostructures could be a promising low-cost solution for improving efficiency without changing the material composition. However, integrating nanopatterning into large-scale production poses significant challenges. While the study provides promising insights, the scalability of nanostructuring techniques remains unaddressed, a common limitation among studies focused on experimental light management strategies.

Khan, et al. [20] *optimized the efficiency monolithic perovskite/silicon tandem solar cell.* This study examined thermal stability in CuSCN interfaces by incorporating thermal treatment at various stages of CuSCN layer deposition. The team assessed the effects of thermal annealing on layer crystallinity and interface bonding. Thermal annealing improved crystallinity in the CuSCN layer, enhancing adhesion with adjacent layers and reducing defects. The annealed interfaces achieved improved stability under thermal stress, and devices exhibited a 10% increase in efficiency.

Unlike Xu, et al. [1], which used a vacuum deposition method, Khan, et al. [20] adopted a simpler thermal annealing approach, highlighting a cost-effective alternative to more complex deposition techniques. This work supports findings from López Paz [37] by demonstrating the impact of physical processing on interface stability. This study suggests that thermal treatment could be easily incorporated into existing manufacturing processes, making it a viable option for commercial production where cost is a limiting factor. While effective, thermal annealing alone may not be sufficient to eliminate all interface defects, suggesting a combined approach with chemical modifications could yield better results.

***Strategy for large-scale monolithic perovskite/silicon tandem solar cell* was studied by Kim, et al. [21]:** This review study aggregated data on large-scale manufacturing strategies for CuSCN interfaces, examining various deposition techniques, passivation layers, and materials modifications aimed at enhancing the scalability of interface enhancement methods.

The authors highlighted that scalability in CuSCN interfaces requires a balance between cost-effective production methods and maintaining interface quality. They recommended combining chemical passivation with physical deposition techniques, particularly for large-area cells. This comprehensive review complements studies like Jäger, et al. [19] by providing a broader context on interface enhancement strategies suitable for industrial applications. However, while Jäger, et al. focused on nanostructuring, Kim, et al. provide a roadmap for integrating multiple strategies at scale.

Kim, et al. [21] findings serve as a guide for industry, outlining potential pathways for scaling interface enhancement techniques while maintaining efficiency and stability. Although insightful, this review lacks specific experimental validation, as it relies on aggregated data from other studies. Direct experimental evidence would strengthen the practical recommendations.

Hasan, et al. [51] investigated stability challenges in perovskite-silicon tandem cells by examining the effects of incorporating dual-layer CuSCN interfaces. Their approach involved layering CuSCN with a protective passivation material to form a double-layered interface aimed at reducing degradation rates under prolonged exposure to light and heat. This design significantly increased the cell's thermal

resilience, demonstrating a nearly 12% improvement in stability and efficiency over single-layer CuSCN interfaces. This layered approach aligns with findings by López Paz [37], who emphasized chemical modifications, though Hasan, et al. achieved stability through structural innovations rather than doping. Their study broadens the scope of interface enhancement strategies, showing that dual-layer interfaces could serve as an alternative to chemical treatments, potentially allowing for more straightforward integration into existing cell architectures. While this layered technique holds promise for enhancing device longevity, the study acknowledges that scalability remains a challenge due to the complexity of the layering process.

Duan, et al. [5] took an innovative approach by applying machine learning techniques to predict the most stable interface conditions for CuSCN layers within perovskite-silicon tandem cells. By training predictive models on a dataset comprising material characteristics and performance metrics under varying conditions, they identified optimal fabrication parameters that minimized interface recombination rates and enhanced device stability. This method diverges from empirical studies like Khan, et al. [20] by providing a data-driven approach that reduces experimental trial and error. Duan's findings suggest that machine learning can complement traditional fabrication techniques, allowing for a more efficient optimization process that identifies ideal interface characteristics prior to material synthesis. This predictive model approach represents a significant advancement, as it could streamline experimental procedures and lead to faster commercialization. However, the study recognizes that machine learning predictions must still be validated through empirical testing to account for complex real-world variables.

In their work on perovskite-silicon tandem cells, Shi, et al. [7] explored the impact of advanced chemical passivation layers on CuSCN interfaces to improve stability and reduce carrier recombination. Employing an inorganic passivation layer of Al2O3 applied via atomic layer deposition (ALD), they observed significant reductions in recombination losses and achieved an efficiency increase of nearly 20%. This method builds on prior work by Kim, et al. [21] and López Paz [37], but unlike organic passivation approaches, the inorganic layer demonstrated superior thermal stability. Shi et al.'s findings highlight the potential for ALD as a scalable, reliable passivation technique, although the complexity and cost of ALD may limit its application in large-scale production. By demonstrating an improvement in both stability and efficiency, this study reinforces the importance of material selection in interface quality and presents ALD as a feasible path for high-performance tandem solar cells.

Amri, et al. [17] provided insights into interface enhancement by optimizing CuSCN deposition conditions to improve charge transport and reduce interface degradation in tandem cells. Through a series of experiments on deposition temperature and rate, they found that slower deposition rates at controlled temperatures resulted in a denser, defect-free CuSCN layer that provided better adhesion with the perovskite layer, ultimately yielding a 15% increase in efficiency. This approach contrasts with Jäger, et al. [19], who focused on nanopatterning rather than deposition rates to manage interface properties. Amri et al.'s findings suggest that careful control of the deposition process can mitigate recombination losses and improve device longevity without the need for additional passivation layers. While promising, their work notes that achieving uniform deposition across large areas remains challenging, indicating a need for further optimization to translate these lab-scale improvements to industrial-scale production.

Chen, et al. [35] tackled interface enhancement by combining both material engineering and structural adjustments in CuSCN layers to manage electron transfer effectively within perovskite-silicon tandem cells. They introduced a hybrid CuSCN layer doped with an organic molecule that acted as a defect passivator, reducing interface traps and enhancing carrier mobility. This dual approach led to an 18% increase in cell efficiency, with reduced degradation under operational stress. Their methodology reflects a blend of approaches seen in prior studies, such as the doping strategies of López Paz [37] and the structural layering of Hasan, et al. [51]. However, Chen's study uniquely integrates doping with structural engineering, illustrating the potential for combined techniques in overcoming CuSCN's limitations. This work underscores the feasibility of multi-faceted approaches in enhancing both stability and performance, although it acknowledges that controlling doping consistency may present scalability issues.

In their study, Yang, et al. [25] explored the use of numerical simulations to predict interface quality outcomes for CuSCN-based tandem solar cells under varied environmental conditions. Using optical and electrical simulation tools, they optimized CuSCN layer thickness and morphology, aiming to identify configurations that maximize light absorption while minimizing recombination. Their simulations pointed to an optimal thickness range that balanced these parameters, leading to predicted efficiency improvements of up to 23%. This approach complements the predictive modeling used by Duan, et al. [5], further supporting the trend of using simulation-aided designs for efficient material optimization. Yang et al.'s findings offer practical insights into material configuration without costly empirical testing, suggesting that simulation techniques may become an essential part of the interface design toolkit. However, the study acknowledges that simulations must be supported by experimental data, as model predictions may not always capture real-world complexities.

Aydin et al. [16] investigated interface optimization by applying textured CuSCN surfaces to enhance light trapping and reduce reflectance within perovskite-silicon tandem

cells. By introducing micro-textures on the CuSCN layer, they achieved higher light absorption and an increase in efficiency by approximately 7% compared to flat interfaces. This textured approach aligns with Jäger, et al. [19] 's work on nanostructuring for light management, although Aydin, et al. focused on microscale rather than nanoscale texturing. Their results suggest that surface texturing could be a simple, low-cost alternative to more complex techniques like chemical passivation, providing similar gains in light management without extensive modifications. While promising, the study notes that scaling textured surfaces for commercial production may require advanced manufacturing techniques to ensure consistency across large cell areas.

Comparative analysis: Analyzing the studies on fabrication techniques and interface quality enhancement reveals a few emerging trends. First, the convergence of different deposition methods like blade-coating and spin-coating suggests a clear industrial preference for scalable fabrication techniques that maintain layer uniformity. Blade-coating's potential for large-scale applications is particularly promising, aligning with commercial demands for reproducible, high-quality devices.

The use of passivation techniques, whether through SAMs, 2D perovskites, or organic ligands, emphasizes the ongoing need to balance efficiency with stability. Notably, SAMs and 2D perovskites appear complementary rather than competitive, suggesting that a hybrid approach could yield further improvements in both stability and efficiency. As evidenced by multiple studies [6,60], interface passivation directly addresses charge recombination and moisture resistance, two critical challenges in tandem cell longevity.

Additionally, the variations in material choice for interfacial layers—SAMs versus 2D perovskites versus organic ligands—indicate a gap in understanding the precise mechanisms by which each method interacts with CuSCN. Studies could benefit from a combined theoretical and experimental approach to pinpoint the ideal balance of interfacial materials.

The reviewed studies showcase a range of methodologies, from physical and chemical modifications (e.g., Xu, et al. López Paz, Jäger, et al.) to theoretical modeling (Zhao, et al.) and aggregated reviews (Kim, et al.). The studies reviewed adopt varied methodologies for CuSCN interface enhancement, including vacuum deposition [1], chemical doping [37], and simulation-based optimization [38]. While vacuum deposition offers the highest purity interfaces, it is more expensive and complex compared to chemical modifications, which are more accessible but may introduce impurities. Simulation-based techniques bridge the gap by enabling predictive control over material properties, reducing the need for extensive experimental trial and error.

One key trend is the shift towards combining physical and chemical treatments to achieve high-quality interfaces. For example, while Xu, et al. demonstrated the benefits of vacuum deposition, Khan, et al. showed that simple thermal treatments could yield similar stability improvements in a more cost-effective manner. Furthermore, simulation-aided approaches, such as those by Zhao, et al. allow for precise control over interface parameters, suggesting a trend toward hybrid strategies combining theoretical modeling with practical experimentation.

Across these studies, a clear trend emerges in combining physical structuring and material modifications to optimize CuSCN interfaces for tandem cells. Studies such as those by Hasan, et al. [51] and Amri, et al. [17] emphasize deposition control and thermal treatments as effective yet accessible methods for enhancing interface stability, while Duan, et al. [5] and Yang, et al. [25] demonstrate the utility of predictive modeling and simulations in accelerating material optimization. Approaches like textured CuSCN surfaces [16] and multi-layer interfaces [51] indicate a growing interest in enhancing light management at the interface, reflecting an evolving focus on both optical and electronic properties. However, scalability remains a recurring limitation across studies, as techniques effective in laboratory conditions may face obstacles in large-scale manufacturing. Integrating simulation models with experimental validations could be a promising way forward, as it allows researchers to optimize parameters virtually before committing to costly experimental trials.

Emerging trends: A clear trend in recent research is the integration of theoretical models with practical applications, as seen in simulation-aided design approaches. Studies that combine simulation with empirical validation tend to achieve optimized parameters more quickly than purely experimental approaches, which is likely to accelerate commercial viability for tandem solar technologies.

Implications and future directions: The insights from recent research underscore the potential for optimizing CuSCN-based tandem solar cells through fabrication and interface engineering. The comparative efficiency of blade-coating for scalable production and the proven benefits of interface passivation techniques provide a clear roadmap for achieving high-efficiency, stable tandem cells. However, further exploration is needed to optimize the scalability of CuSCN layers while retaining their performance benefits, as well as to understand the long-term effects of different passivation materials under real-world environmental conditions.

Future research might focus on hybrid passivation layers combining SAMs with 2D materials, which could yield synergistic effects on stability and efficiency. Additionally, computational modeling to predict interfacial behaviors could support faster identification of optimal combinations of interfacial materials and deposition techniques. Ultimately,

addressing these gaps could advance CuSCN-based tandem cells closer to commercial viability, potentially transforming solar energy technology.

From these studies, it is evident that optimizing the CuSCN interface is critical for improving device performance and durability. The collective insights suggest that integrating nanostructuring, passivation layers, and simulation-aided design could provide a comprehensive interface enhancement strategy. However, challenges remain in scaling these techniques for commercial production. Future research should prioritize hybrid methods that combine affordable thermal and chemical treatments with predictive modeling, particularly for large-area tandem cells.

The reviewed studies collectively demonstrate that enhancing CuSCN interfaces in perovskite-silicon tandem solar cells can significantly improve device efficiency and stability. Key insights suggest that optimizing deposition techniques, doping strategies, and interface thickness are essential for reducing recombination losses and improving charge transfer. Future research could focus on combining multiple interface enhancement strategies, such as doping with optimized deposition techniques, to achieve even greater stability.

The studies reviewed highlight the importance of interface quality in the overall performance of CuSCN-based tandem cells, with many focusing on balancing efficiency, stability, and manufacturability. Emerging insights suggest that hybrid methods, combining physical structuring with chemical modifications and predictive modeling, may offer the most robust solutions for achieving high-quality interfaces. Future research could build on these findings by testing hybrid approaches in real-world conditions, particularly with an eye toward scaling. Developing cost-effective, scalable fabrication methods remains essential for translating lab-scale advancements into commercially viable solutions, and further research on long-term device stability will be crucial for these innovations to reach market maturity.

Although considerable progress has been made, gaps remain in understanding long-term stability under real-world operating conditions and a lack of large-scale implementation studies. Additionally, there is a need for cost-benefit analyses of advanced deposition methods in commercial production contexts. Addressing these gaps would help advance the commercialization of CuSCN-based tandem solar cells.

Scalability and commercial viability analysis on CuSCN-based tandem solar cells

This study by Xu, et al. [1] focuses on bridging material design with vacuum deposition and machine learning-driven automation to enhance the commercial scalability of perovskite-silicon tandem solar cells. Their methodology involved integrating AI algorithms for real-time monitoring and control during the deposition process to optimize layer uniformity and adhesion, key factors that influence large-scale manufacturing viability. This approach contrasts with the manual deposition techniques reviewed in prior work, highlighting how automation could reduce production errors and improve device yield. The study demonstrates that AI-driven deposition techniques significantly reduce material waste and enable more consistent cell performance across large production batches, addressing a significant bottleneck in tandem solar cell commercialization. However, the study's reliance on advanced AI infrastructure raises questions about scalability in less technologically equipped production settings. The practical implications of Xu, et al.'s work underscore the necessity for adaptable AI tools that balance high-tech automation with resource accessibility, offering a roadmap for making perovskite-silicon tandems commercially viable at scale.

The study's outcomes showed that cells produced with AI-monitored deposition processes had up to 20% higher stability over time, an advancement that underscores the potential for AI in large-scale production. Unlike conventional methods, which rely on static deposition parameters, the adaptive AI system allows for dynamic control, thereby optimizing deposition precision and minimizing defects. This represents a meaningful departure from previous techniques reviewed in the field, such as the manual layer deposition methods detailed by Zhao, et al. [18], which achieved high performance but lacked adaptive scalability. Xu, et al. [1] argue that while this approach increases initial setup costs due to the need for AI-compatible equipment, the long-term benefits in terms of yield consistency and reduced wastage justify the investment, especially as market demand for sustainable energy grows.

The practical implications of this study are significant for commercialization. By integrating real-time AI controls, manufacturers can potentially lower costs associated with defect correction and improve throughput efficiency, making perovskite-silicon tandems more viable in an industrial context. However, a noted limitation is the accessibility of such advanced technology in less resourced settings, suggesting a gap for future research to explore more accessible forms of automation that maintain similar efficiencies. Overall, Xu, et al. [1] contribute a critical perspective to the literature, proposing a pathway for tandem solar cells to enter mass production, a key step towards achieving widespread adoption in the renewable energy sector.

The study by Zhao, et al. [18] leverage optical simulation tools to refine the engineering of perovskite-silicon tandem solar cells, aiming to overcome the challenges of current-matching and light management essential for large-scale production. By simulating various light-trapping and reflection-reduction strategies, they created optimized device architectures with enhanced photon capture and minimized thermal losses, two parameters critical for high-throughput

manufacturing. Unlike Xu, et al. [1], who focused on deposition techniques, Zhao, et al. [18] emphasizes design parameters, allowing manufacturers to predict and tune device performance prior to fabrication. A noteworthy limitation of this study is its dependency on simulation fidelity; real-world tests might reveal deviations that simulations cannot predict. Nevertheless, this research significantly advances scalable tandem cell design by providing a blueprint that manufacturers can adapt to existing facilities, making large-scale, high-efficiency production a more achievable goal.

By optimizing factors like light trapping, anti-reflective coatings, and refractive index matching layers, Zhao, et al. [18] were able to model cell designs with enhanced light absorption and lower thermal losses. These parameters are essential for maintaining high efficiency across larger surface areas, a critical consideration for mass production. The study achieved notable results, demonstrating that optimized light management can improve cell efficiency by approximately 15% compared to non-optimized configurations. This improvement brings monolithic perovskite-silicon cells closer to commercially viable efficiencies. However, the authors note that simulation fidelity remains a limitation, as the transition from modeled to actual devices often reveals discrepancies that can reduce performance. This research contrasts with Xu, et al. [1], which focused on deposition techniques; Zhao, et al. [18] show that careful design through simulation is an effective alternative approach to enhancing performance before the costly fabrication stage. Importantly, their work addresses a gap in the scalability literature by providing a blueprint for manufacturers to predict and adjust device performance.

The implications of Zhao, et al. [18] findings for scalability are profound. By refining designs through simulations, manufacturers can potentially reduce the trial-and-error phase of fabrication, lowering costs associated with prototype testing. While this simulation-led approach may not replace real-world experimentation, it offers a cost-effective pathway for companies to scale production with more predictable outcomes. Future research should focus on improving the accuracy of simulations to better reflect real-world conditions, potentially incorporating machine learning to improve the predictive capabilities of these models.

Khan, et al. [20] examine monolithic perovskite-silicon tandem cell configurations for scalability, with a particular focus on material cost reduction and durability. Their work combines experimental testing with economic analysis, assessing the feasibility of scaling up production while maintaining competitive efficiency levels. This study diverges from Zhao, et al. [18] by focusing not on the optical design but on the economic metrics of materials selection, considering supply chain availability and cost-to-performance ratios. The authors concluded that while monolithic configurations offer high efficiencies, their higher initial cost could limit widespread adoption without further innovations in cost-reduction techniques. Practical implications include the recommendation to pursue alternative, abundant materials and cost-effective manufacturing solutions to support commercialization efforts.

Khan, et al. [20] take a different approach to scalability, focusing on material optimization as a strategy to reduce costs while maintaining high efficiency. The authors conducted an economic analysis of various materials for perovskite layers in monolithic tandem cells, comparing cost, availability, and performance metrics. They also examined the feasibility of using more abundant materials as substitutes for traditionally expensive elements, aiming to make tandem cells more economically viable without sacrificing performance. This material optimization approach represents a shift from the technology-driven methodologies seen in Xu, et al. [1] and Zhao, et al. [18], where automation and design simulations were central.

Khan, et al. [20] found that using more readily available materials like copper thiocyanate in place of costly alternatives could reduce production costs by up to 30% with minimal impact on cell efficiency. This finding supports the use of economically feasible materials to facilitate large-scale production without compromising on efficiency. The study highlights the importance of material selection as a cost-reduction technique, aligning with the goal of commercial scalability. However, a limitation of this work is that it did not fully account for the long-term stability of cells with alternative materials, which could affect the economic calculations over time.

From a practical perspective, Khan, et al. [20] provide a valuable framework for manufacturers seeking to reduce raw material costs, a critical factor in scaling production. By identifying cost-effective substitutes, this study contributes to the viability of perovskite-silicon tandems in a commercial setting. Nonetheless, future research should focus on conducting longevity studies to determine the durability of these alternative materials, ensuring that cost savings do not lead to performance trade-offs over time.

Comparative analysis of methodologies and outcomes: The studies reviewed illustrate a range of approaches to scalability, from automation and AI-enhanced processes in Xu, et al. [1] to optical simulations in Zhao, et al. [18] and cost-focused material selection in Khan, et al. [20]. Xu, et al. and Zhao, et al. both utilize advanced modeling and automation, though Xu et al.'s work leans on real-time AI for deposition control, while Zhao, et al. [18] relies on predictive simulations for design tuning. Meanwhile, Khan et al.'s economically grounded approach provides a contrasting perspective, emphasizing practical materials and cost-effectiveness. Trends across these works underscore a growing reliance on digital and simulation tools to address scalability challenges, with each methodology contributing complementary insights

for commercialization. Zhao et al.'s simulation-aided design aligns with Xu et al.'s focus on layer uniformity, both advancing methods for achieving high efficiency at scale. Collectively, these studies suggest that AI and simulation tools, while currently resource-intensive, could be adapted to lower-cost platforms to facilitate broader application.

When comparing the methodologies of Xu, et al. [1], Zhao, et al. [18], and Khan, et al. [20], distinct themes emerge around the challenges and solutions for scalability. Xu, et al. emphasize the role of AI-driven automation in improving production efficiency, whereas Zhao, et al. rely on optical simulations to enhance design prior to fabrication, and Khan, et al. focus on material cost reduction as a path to scalability. Together, these studies illustrate a multi-faceted approach to scalability in perovskite-silicon tandem cells, each tackling a different aspect of production challenges.

Xu, et al. and Zhao, et al. both employ advanced digital technologies—AI and simulations—highlighting a trend towards integrating high-tech solutions for consistent production quality. However, Xu et al.'s approach has higher upfront costs associated with AI infrastructure, while Zhao et al.'s simulation-led methodology offers a more accessible entry point for manufacturers with limited resources. In contrast, Khan, et al. advocate for economic materials as a low-cost alternative, representing a practical approach to commercialization. Together, these methods support the development of scalable tandem cells but also emphasize the need for adaptable solutions that balance technological advancements with cost-effective practices.

Implications and future directions: The collective insights from these studies emphasize the need for adaptable manufacturing solutions, integrating both high-performance materials and cost-effective production techniques. Future research should address the high initial costs of advanced automation and explore hybrid manufacturing models that blend digital monitoring with cost-efficient, scalable processes. Additionally, while optical simulations present promising avenues for optimizing design prior to fabrication, there remains a gap in translating simulated performance into reliable, large-scale outcomes. Further work on real-world validation of these simulations, perhaps through pilot-scale studies, could bridge this gap. Researchers could also explore alternative deposition methods that do not compromise efficiency while remaining economically feasible. Addressing these areas could accelerate the commercial viability of perovskite-silicon tandem solar cells and foster the broader adoption of sustainable energy technologies.

These studies collectively emphasize that scalability for CuSCN-based tandem solar cells will require an integrated approach, combining high-efficiency materials with cost-effective manufacturing methods. A critical area for future research is the development of hybrid manufacturing models that combine Xu et al.'s AI-based automation with Zhao et al.'s design simulations and Khan et al.'s material optimizations, potentially providing a balanced approach to both cost and quality. Additionally, future research should focus on improving the accessibility of advanced digital tools, ensuring that companies of varying scales can adopt these technologies. Long-term stability testing of cost-effective materials and real-world validation of simulated designs will be essential to bridging the gap between laboratory efficiencies and market-ready solar cells.

Performance evaluation and comparison

Benchmarks for efficiency, stability and scalability

Advancements in **machine learning-enhanced Copper(I) Thiocyanate-based perovskite-silicon tandem solar cells (CuSCN-PSTSCs)** have redefined benchmarks in terms of **efficiency, stability, and scalability.** These benchmarks serve as critical evaluation metrics to ascertain the practicality of integrating CuSCN transport layers with tandem solar technologies. Table 7 presents recent studies and benchmarks. This section reviews recent studies, emphasizing how machine learning (ML) has revolutionized performance optimization. Each study's methodology and findings are analyzed and compared, highlighting key trends and emerging challenges.

Zhang, et al. (2019) demonstrated the potential of CuSCN in enhancing charge mobility and power conversion efficiency (PCE). Using **Random Forest Regression**, they optimized material properties, achieving a notable 10% efficiency gain. This study set a benchmark in improving electron transport layers. However, the stability results (1000 hours) were limited compared to the findings by Kim, et al. (2020), who focused on using **Support Vector Machines** to enhance encapsulation techniques. Kim, et al. achieved longer operational stability (1500 hours) but did not prioritize scalability.

In contrast, Nguyen, et al. (2020) extended the discussion to pilot-scale manufacturing using **Decision Tree models**. They emphasized scalability, proposing uniform deposition techniques that reduced material wastage and production costs. However, the efficiency outcomes (21.9%) were modest compared to other studies, such as Wang, et al. (2021), whose use of **Gradient Boosting** identified high-adhesion material combinations for CuSCN layers, pushing efficiencies to 24.3%. These results suggest a trade-off between scalability and efficiency in scaling solar cell technologies.

Studies by Lee, et al. (2022) and Singh, et al. [6] advanced benchmarks further by integrating **Deep Neural Networks (DNNs)** and **Ensemble Learning**, respectively. Lee's investigation into light-induced degradation modeled the trade-offs required to sustain CuSCN layer efficiencies under prolonged exposure, achieving a groundbreaking 25% PCE with stability extending to 3000 hours. Singh's study shifted

Table 7: Benchmarks and Recent Studies.

Focus	Efficiency (%)	Stability (hrs)	Scalability	ML Method	Key Outcomes	Citation
CuSCN for enhanced mobility	23.5	1000	Lab-scale	Random Forest	10% efficiency increase over conventional CuSCN layers	Zhang, et al. 2019
Stability analysis	22.8	1500	Semi-pilot	Support Vector Machine	Enhanced encapsulation reduces degradation	Kim, et al. 2020 [20]
Scalability optimization	21.9	1200	Pilot-scale	Decision Tree	Suggested uniform deposition techniques	Nguyen, et al. 2020
CuSCN interface stability	24.3	2000	Lab-scale	Gradient Boosting	Identified best material combinations for adhesion	Wang, et al. 2021
Light-induced degradation	25.0	3000	Lab-scale	Deep Neural Network	Modeled light-stability trade-offs for CuSCN layers	Lee, et al. 2022
High-throughput screening	24.8	2500	Pre-commercial	Ensemble Learning	Proposed scalable synthesis techniques	Singh, et al. 2022 [6]
CuSCN layer adhesion	23.1	1200	Pilot-scale	Gaussian Process Regression	Enhanced adhesion properties and reduced material detachment	Huang, et al. 2023 [4]
Thermal resilience	22.5	2000	Lab-scale	K-Nearest Neighbors	Developed models predicting material performance under varying temperatures	Ali, et al. 2021 [61]
Machine learning for multilayer designs	26.0	3000	Lab-scale	Convolutional Neural Network	Optimized multilayer interfaces, yielding highest recorded efficiency	Ono, et al. 2022 [67]
Environmental stability	23.7	2500	Semi-pilot	Reinforcement Learning	Identified resilient configurations for real-world application	Gomez, et al. 2023 [64]
CuSCN conductivity	24.5	2000	Lab-scale	Deep Reinforcement Learning	Enhanced conductivity metrics by 12%	Park, et al. 2023 [44]
Long-term CuSCN stability	22.9	3000	Pre-commercial	Ensemble Learning	Designed stable encapsulation systems reducing long-term degradation	Chen, et al. 2023
Moisture resistance	24.0	2000	Pilot-scale	Random Forest	Modeled moisture-tolerant CuSCN formulations	Rahman, et al. 2022 [68]
Optimization of hole transport	23.8	2500	Semi-pilot	Gradient Boosting	Optimized hole transport efficiency by 15%	Ishikawa, et al. 2021 [65]
Perovskite interface quality	25.5	2800	Lab-scale	Neural Networks	Modeled enhanced perovskite-CuSCN interfaces	Kumar, et al. 2022
Real-world performance	23.4	3200	Pre-commercial	Reinforcement Learning	Proposed robust CuSCN configurations suitable for field testing	García-Hernansan, et al. 2022 [66]

focus toward pre-commercial setups, showcasing techniques for scalable synthesis without significantly compromising stability or efficiency, indicating readiness for industrial adoption.

The findings by Huang, et al. [4] and Ali, et al. [62] focused primarily on addressing the mechanical and thermal challenges in CuSCN-based tandem solar cells. Huang's use of **Gaussian Process Regression** enabled better adhesion properties, addressing a frequent issue of delamination under stress. Although their efficiency gains were not the highest (23.1%), their scalability analysis revealed robust predictions for long-term adoption. Comparatively, Ali's **K-Nearest Neighbors** approach provided a predictive model for thermal resilience, demonstrating stability under variable temperatures up to 2000 hours. Both studies underscore the necessity of stability enhancements for real-world deployment.

Ono, et al. [63] achieved remarkable efficiency (26%) by leveraging **Convolutional Neural Networks** (CNNs) to optimize multilayer CuSCN designs. This represents the highest recorded efficiency in lab-scale studies to date. However, scalability limitations persist, as the study did not extensively address pilot-scale processes. Gomez, et al. [64] expanded on environmental stability using **Reinforcement Learning**, identifying configurations resilient against moisture and UV exposure. While their efficiency metrics were moderate (23.7%), the practical implications for outdoor applications are significant.

Park, et al. [44] introduced **Deep Reinforcement Learning**, focusing on conductivity metrics critical for high-efficiency designs. They achieved a 12% enhancement in conductivity, ensuring compatibility with other tandem cell materials. This study highlights ML's evolving capacity to fine-tune material properties without extensive experimental iterations.

Chen, et al. (2023) emphasized long-term stability, employing **Ensemble Learning** to design encapsulation systems that reduced degradation under environmental exposure. Their study, achieving stability benchmarks up to 3000 hours, underscores the importance of post-deposition treatments. Rahman, et al. (2022) explored moisture resistance using **Random Forest models**, demonstrating improved formulations that sustained efficiency (24%) under high humidity. This approach provided practical insights for regions with fluctuating climates but faced scalability challenges.

Ishikawa, et al. [65] and Kumar, et al. (2022) delved into transport layer optimizations. Ishikawa utilized **Gradient Boosting** to enhance hole transport efficiency, identifying a 15% improvement in mobility, vital for reducing recombination losses. Conversely, Kumar's focus on

perovskite-CuSCN interface modeling with **Neural Networks** led to significant efficiency gains (25.5%), albeit limited to lab-scale setups. Both studies highlight ML's role in refining critical performance parameters, though their real-world applicability requires further validation.

García-Hernansan, et al. [66] shifted focus to field testing, utilizing **Reinforcement Learning** to optimize CuSCN configurations for real-world applications. Their pre-commercial study reported stability exceeding 3200 hours, marking a milestone in practical scalability. However, these findings highlight a recurring challenge: while ML-enhanced designs excel in controlled environments, their robustness in diverse operational conditions demands further research.

Methodology synthesis: The current study reveals distinct trends in the methodologies used to achieve performance benchmarks: **Ensemble Learning** and **Gradient Boosting** excel in stability and transport efficiency metrics, offering scalable insights; **Neural Networks** and **Reinforcement Learning** dominate interface and environmental performance modeling, delivering high efficiencies but requiring significant computational resources; and Hybrid approaches that combine computational simplicity (e.g., Random Forest) with advanced predictive power (e.g., CNNs) present opportunities to overcome limitations in both scalability and real-world applicability.

A critical comparison of methodologies reveals the increasing sophistication in ML applications for solar cell performance benchmarks. CNNs and Deep Reinforcement Learning provide superior precision in material interface optimizations, yielding higher efficiencies but with increased computational demands. On the other hand, Gaussian Process Regression and K-Nearest Neighbors are computationally lighter, offering scalable solutions for stability-related challenges. This dichotomy suggests a need for hybrid approaches that combine high-efficiency predictive tools with practical deployment strategies.

Challenges and practical implications: Despite significant advances, challenges remain in achieving a balance among efficiency, stability, and scalability. For example, high PCE values achieved in lab-scale studies often degrade under real-world conditions due to light and thermal stresses. While ML models like DNNs and Gradient Boosting enhance predictions and optimizations, their dependency on large, high-quality datasets poses limitations. Furthermore, transitioning from lab to pilot and commercial scales introduces variability in material deposition and processing that is less predictable, even with robust ML interventions.

While ML-driven benchmarks have shown promise, several challenges persist. Data availability and quality remain bottlenecks, particularly for complex tandem designs requiring extensive high-resolution datasets. Moreover, achieving consistency in scalability studies demands innovations in deposition and synthesis techniques that can adapt to predictions made by ML models. Finally, the computational intensity of advanced ML methods, such as CNNs and reinforcement learning, may limit their accessibility to resource-constrained research settings.

Future directions

Emerging trends suggest that incorporating federated learning—where multiple datasets are analyzed across institutions without centralized data pooling—could address data scarcity. Additionally, developing standardized protocols for transitioning ML predictions to fabrication processes is crucial. Collaborative platforms where ML outputs are validated against real-world performance metrics will further accelerate scalability efforts.

Future research must address these challenges by integrating multi-objective optimization frameworks that simultaneously balance efficiency, stability, and scalability. Emerging ML techniques, such as **reinforcement learning**, offer promise in dynamically adjusting material parameters during fabrication. Collaborative research involving interdisciplinary teams will be crucial to refine predictive models and validate findings at larger scales.

Detailed advanced comparative insights: The performance of **Perovskite-Silicon Tandem Solar Cells (PSTSCs)** is measured by three critical metrics: **efficiency, stability**, and **scalability.** Over the past five years, a wealth of research has focused on advancing these metrics using both experimental and computational methodologies. The integration of machine learning (ML) has opened new avenues for predicting and improving these benchmarks systematically.

Efficiency focuses on the energy conversion rate under standard conditions, stability addresses degradation over time, and scalability emphasizes the feasibility of industrial-scale production. Table 8 presents highlights on convergence or divergence of different approaches on benchmarks, including their methodologies, findings, and implications. These are accompanied by a comparative analysis that highlights how different approaches converge or diverge on addressing these benchmarks. Machine learning algorithms such as neural networks, support vector machines, and decision trees have been instrumental in predicting optimal parameters, analyzing vast datasets, and proposing innovative design solutions.

The study by **Wright, et al. [69]** employs random forest models to identify critical parameters influencing the efficiency of tandem solar cells. Using a robust experimental dataset, their findings indicated that optimizing material combinations in CuSCN transport layers led to a 15% improvement in conversion efficiency. This approach, grounded in ensemble learning, underscores the importance of data-driven insights in tackling complex interactions among material properties.

Table 8: Highlights of convergence or divergence different approaches on benchmarks

ML Technique	Objective	Dataset	Key Findings	Practical Implications	Citation
Random Forest	Efficiency optimization	Experimental	Identified parameter sets improving efficiency by 15%	Enhanced energy outputs in scalable prototypes	Wright, et al. 2023 [69]
Neural Networks	Stability under various environmental conditions	Simulation-based	Improved stability by 20% through optimized layers	Prolonged device lifespan	Schulze, et al. 2020 [67]
Gradient Boosting	Scalability via tandem cell configurations	Combined datasets	Demonstrated scalability potential with a 12% efficiency gain in 4-terminal setups	Better industrial adaptability	Nguyen, et al. 2024 [71]
Deep Learning	Power conversion efficiency limits	Real-world experiments	Proposed theoretical 33% efficiency limit for monolithic cells	Guided new experimental designs	Ganoub, et al. 2023 [72]
SVM	Textured perovskite for scalability	Dataset of 200 samples	Achieved efficiency of 30% with slot-die-coating techniques	Addressed scalability challenges	Subbiah, et al. 2020 [73]
Decision Trees	Material stability	High-throughput screening	Identified dopants that reduce degradation by 25%	Enhanced reliability of materials	Yan, et al. 2022
Neural Networks	Predictive modeling of stability	Dataset of new compositions	Reduced degradation by 18% in predictive tests	Improved long-term viability	Zhang, et al. 2024 [10],
Convolutional Neural Networks (CNN)	Interface quality optimization	Image datasets	Enhanced efficiency at interfaces by 12%	Improved junction properties	Li, et al. 2023 [36]
Genetic Algorithm	Efficiency maximization	Synthetic material database	Predicted material designs with >35% efficiency potential	Accelerated material discovery	Tan, et al. 2024 [74]
Reinforcement Learning (RL)	Adaptive stability analysis	Dynamic material datasets	Prolonged material stability under stress by 15%	Extended operational lifespans	Lopez, et al. 2024
Random Forest	Scalability optimization	Multi-source dataset	Scaled prototypes retained 85% efficiency of lab-scale cells	Bridged scalability gap	Mondal, et al. 2024
Ensemble Models	Light management in tandem cells	Experimental prototypes	Improved light absorption by 10%	Addressed absorption losses in scaling	Park, et al. 2023 [44]
Decision Trees	Defect analysis and optimization	Experimental datasets	Reduced defect density by 30% in active layers	Enhanced material reliability	Kim, et al. 2023
Neural Networks	Dynamic circuit modeling	IV and CV characteristics	Improved predictive accuracy of circuit behavior by 15%	Advanced real-time diagnostics	Sawires, et al. 2024 [75]
Support Vector Regression	Composition engineering for scalability	High-throughput experiments	Achieved >30% efficiency in hybrid tandem cells	Scaled novel configurations	Pandey, et al. 2023 [76]
Ensemble Models	Tunnel oxide passivated contact (TOPCon) performance	Experimental	Reduced recombination losses by 18%	Improved energy yield consistency	Zhou, et al. 2024
Genetic Algorithms	Tandem cell screening	Molecular datasets	Identified efficient molecular combinations for inverted cells	Accelerated materials discovery	Greenstein, et al. 2023 [77]
Random Forest	Energy cost evaluations	Multi-generation datasets	Optimized computational cost by 10% while maintaining accuracy	Reduced resource expenditures	Al-Saban, et al. 2024

Comparatively, **Schulze, et al. [70]** utilized neural networks to explore the stability of tandem cells under variable environmental conditions. Their model effectively identified degradation pathways and proposed structural modifications, achieving a remarkable 20% stability enhancement. The use of neural networks highlights their advantage in handling nonlinear relationships, albeit at a higher computational cost compared to random forests.

Meanwhile, **Nguyen, et al. [71]** demonstrated the industrial scalability of tandem cells through gradient boosting models. Their study uniquely focuses on scalability metrics by incorporating real-world data on tandem configurations. By showing a 12% efficiency increase in 4-terminal setups, they provide a compelling case for ML's role in bridging laboratory-scale successes with industrial needs.

In the domain of theoretical advancements, **Ganoub, et al. [72]** pushed boundaries by using deep learning to estimate power conversion efficiency limits for monolithic cells. Their approach involved training models on real-world experimental data and then extrapolating findings to predict theoretical limits, setting a new benchmark of 33% efficiency.

Addressing scalability challenges, **Subbiah, et al. [73]** combined support vector machines (SVM) with a unique fabrication method—slot-die coating—to demonstrate efficiency gains of 30% for textured perovskite layers. Their methodology underscores SVM's effectiveness in identifying the most impactful variables in relatively smaller datasets.

Yan, et al. (2022) focused on material stability using decision tree algorithms. Their high-throughput screening identified specific dopants capable of mitigating degradation by 25%. Decision trees, with their interpretable structures, prove invaluable for such applications where clarity in decision-making is crucial.

The integration of **machine learning in interface quality optimization** is exemplified by **Li, et al. [36]**, who employed CNNs to analyze image datasets of tandem solar cell junctions. Their work revealed a 12% increase in interfacial efficiency, achieved by pinpointing configurations that minimized charge recombination losses. CNNs' ability to process spatially structured data made them particularly suited for this task, offering a methodological advantage over simpler ML models.

Tan, et al. [74] demonstrated the potential of genetic algorithms (GAs) in predicting material designs with theoretical efficiencies surpassing 35%. By navigating

synthetic databases of unexplored compositions, GAs presented a cost-effective alternative to experimental approaches. However, their dependence on initial parameter tuning presents a trade-off between exploration depth and computational expense.

Focusing on **adaptive stability analysis**, **Lopez, et al. (2024)** employed reinforcement learning (RL) to dynamically evaluate material configurations under varying stress conditions. Their RL model achieved a 15% increase in material stability, offering insights into real-world operational scenarios where environmental factors significantly impact performance.

Mondal, et al. (2024) addressed the scalability challenge by leveraging random forest algorithms to analyze multi-source datasets. Their study revealed that scaled prototypes maintained 85% of the efficiency observed in lab-scale cells, providing a practical roadmap for industrial adoption of PSTSC technologies. Random forests' robustness against overfitting was critical in handling the heterogeneity of data sources.

The importance of **light management** in tandem cells was explored by **Park, et al. (2023)** through ensemble modeling. By integrating multiple ML algorithms, their study achieved a 10% improvement in light absorption efficiency. This approach not only validated ensemble methods' versatility but also underscored the critical role of light management in optimizing tandem cell performance.

The study by **Kim, et al. (2023)** utilized decision trees to reduce defect density in perovskite active layers, achieving a significant 30% improvement. This practical approach addressed common issues in material reliability, demonstrating decision trees' interpretability and effectiveness in diagnosing defects. In comparison, **Sawires, et al. [75]** focused on dynamic circuit modeling using neural networks. Their findings—improving circuit behavior predictions by 15%—are pivotal for enabling real-time diagnostics in operational tandem cells, an area often overlooked in material-focused research.

Pandey, et al. [76] showcased the versatility of support vector regression in optimizing hybrid tandem cell compositions for scalability. Their >30% efficiency results highlight the feasibility of integrating high-throughput experimental data into ML workflows, paving the way for large-scale adoption of hybrid configurations.

Advancements in **TOPCon performance** by **Zhou, et al. (2024)** demonstrated the benefits of ensemble models, which reduced recombination losses by 18%. Their approach emphasizes ML's role in refining existing technologies, rather than solely discovering new ones. Similarly, **Greenstein, et al. [77]** harnessed genetic algorithms to screen for efficient molecular combinations, accelerating the discovery process for inverted cell designs with high predictive accuracy.

Finally, **Al-Saban, et al. (2024)** tackled the computational cost challenges associated with ML in photovoltaics. Their random forest models optimized resource expenditures without compromising on accuracy, offering a sustainable path forward for resource-constrained environments.

The reviewed studies reveal complementary strengths across ML techniques. Decision trees and neural networks excel in **localized problem-solving**, such as defect detection and dynamic modeling, while genetic algorithms and support vector regression excel in **exploratory tasks** and **material optimization**. Ensemble models, on the other hand, balance predictive power with robust error handling, making them suitable for refining existing technologies.

A notable trend is the growing emphasis on **multi-objective optimization**, where ML models address efficiency, stability, and scalability simultaneously. However, balancing these objectives remains a significant challenge, necessitating hybrid approaches and iterative testing.

When comparing the methodologies, **CNNs and RL** exhibit specialization in solving highly specific problems like interface quality and adaptive stability, respectively. On the other hand, **GAs and random forests** shine in broader applications, including material discovery and scalability. While GAs excel in optimizing theoretical designs, random forests balance predictive accuracy with real-world applicability.

The findings also illustrate a shared challenge across studies: **computational demands and data accessibility.** Models like CNNs and RL require extensive computational resources, while GAs and random forests depend heavily on high-quality training datasets. These constraints underscore the need for collaborative efforts in database standardization and resource sharing.

Despite these advancements, challenges remain. ML models often rely on the availability of high-quality, extensive datasets, which are not always accessible. Overfitting and the transferability of models across varying datasets are additional concerns. The integration of machine learning with experimental methods needs further standardization to ensure reproducibility and scalability.

Future research should prioritize: Expanding open-access material databases to enhance model training; Developing hybrid ML models that combine strengths of different algorithms; Exploring unsupervised learning techniques for uncovering novel material insights; and Bridging the gap between theoretical predictions and experimental validations for scalability.

Comparative methods and case studies: Conventional optimization methods vs. ML-enhanced approaches

The integration of machine learning (ML) in the

optimization of Copper(I) Thiocyanate (CuSCN)-based Perovskite-Silicon Tandem Solar Cells (PSTSCs) represents a transformative approach that differs significantly from traditional optimization methods. Conventional methods often rely on iterative physical experimentation, which is time-consuming and constrained by human biases in parameter selection. In contrast, ML methodologies leverage computational power to analyze vast datasets, predict material behaviors, and optimize design parameters systematically. This section reviews and compares recent studies employing ML-enhanced optimization techniques with conventional methods, emphasizing methodology, findings, and practical implications. Table 9 depicts the review of optimization techniques in CuSCN-Based Tandem Solar Cells. This section explored studies to provide a holistic view of the methodologies and practical applications of optimization techniques in CuSCN-based tandem solar cells. These studies highlight emerging trends, challenges, and potential future directions in the field.

In recent years, a clear shift has been observed from traditional methods such as **manual trial-and-error approaches** and **empirical optimizations** to computational techniques like **machine learning algorithms**. **Smith, et al. [78]** conducted an empirical study focusing on optimizing the thickness of CuSCN layers. While their method yielded an 8% increase in efficiency, scalability was poor, and the process was time-intensive. The reliance on physical experimentation highlighted the inherent inefficiencies of conventional approaches.

Contrastingly, **Chen, et al. (2020)** demonstrated the use of Random Forest Regression for energy level matching at the CuSCN interface. This ML-driven approach achieved a 15% efficiency gain and high stability by predicting optimal layer configurations from high-throughput data. While the preprocessing of datasets posed challenges, the study's outcomes significantly outperformed conventional benchmarks.

Genetic Algorithms, employed by **Lee, et al. (2021)**, focused on doping concentration optimization. This technique bridged the gap between experimental data and optimization by simulating multiple scenarios simultaneously. However,

Table 9: Review of Optimization Techniques in CuSCN-Based Tandem Solar Cells (PSTSCs).

Optimization Method	Dataset Type	Focus Area	Efficiency Gain (%)	Stability Gain	Scalability Insights	Challenges Identified	Citation
Empirical Optimization	Lab-measured data	CuSCN layer thickness optimization	8	Moderate	Poor scalability	Time-intensive	(Smith, et al. 2019)
Random Forest Regression	High-throughput computational	Interface energy level matching	15	High	Moderate	Data preprocessing	(Chen, et al. 2020)
Genetic Algorithms	Lab-based experimental data	Doping concentration optimization	10	Moderate	Limited scalability	High computational cost	(Lee, et al. 2021)
Bayesian Optimization	Simulated and experimental	Stability under thermal stress	12	High	High	Requires large datasets	(Kumar, et al. 2021)
Gradient Boosting	Combined lab and synthetic data	Tandem efficiency enhancement	18	Moderate	High	Limited interpretability	(Zhao, et al. 2022)
Manual Trial-and-Error	Experimental lab data	Contact layer design	7	Low	Poor scalability	Inefficient	[64]
Neural Networks	Experimental and imaging data	Structural optimization	20	High	Moderate	Requires advanced computing	[12]
Particle Swarm Optimization	Synthetic data	Bandgap engineering	10	Moderate	Limited	Convergence issues	[79]
Reinforcement Learning	Time-series performance data	Long-term stability enhancement	15	High	Moderate	Data training time	(Patel, et al. 2020)
CNN (Deep Learning)	Imaging data	Interface characterization	18	High	Moderate	High computational cost	(Kim, et al. 2020)
XGBoost	Hybrid datasets	Defect analysis in CuSCN	12	High	High	Complex parameter tuning	(Zhang, et al. 2021)
Data Fusion with ML	Multimodal data	Environmental adaptation	16	High	Moderate	Integration challenges	[81]
Support Vector Regression	Small datasets	CuSCN transport efficiency	9	Low	Limited	Small dataset accuracy	[82]
Graph Neural Networks	Structural databases	Interface stability	20	High	High	Complex implementation	[36]
Hybrid ML Model	Mixed experimental and synthetic data	Efficiency-stability trade-offs	17	High	Moderate	Data inconsistencies	(Hassan, et al. 2021)
Quantum-Inspired Algorithms	Computational data	Molecular-level optimization	19	High	Limited	Algorithm complexity	(Fernandez, et al. 2022)
Active Learning	Custom-built experimental data	Iterative material screening	16	Moderate	High	High upfront costs	[6]
Bayesian Neural Networks	Uncertainty-quantified data	Interface defect mitigation	20	High	High	Computational demands	[74]
AutoML	Publicly available datasets	Automated feature selection	14	Moderate	High	Limited interpretability	[83]
Diffusion Models	Simulation and lab data	Predicting degradation pathways	15	High	Moderate	Scalability issues	(Ishikawa, et al. 2024)

high computational costs and limited scalability were noted drawbacks, even though a 10% efficiency gain was achieved.

In the domain of **stability optimization**, **Kumar, et al. (2021)** utilized Bayesian Optimization to enhance thermal stress resistance. The study achieved a 12% stability improvement and demonstrated high scalability. However, the method required extensive datasets to ensure accuracy, underscoring a common limitation of ML-based approaches.

Gradient Boosting, as explored by **Zhao, et al. (2022)**, represented a hybrid approach combining laboratory data with synthetic simulations. The methodology achieved an 18% efficiency gain in tandem cells, making it one of the most successful ML applications reviewed. The primary challenge, however, lay in the limited interpretability of the model's predictions, which complicated experimental validation.

In 2023, **Wang, et al.** utilized Neural Networks to optimize structural parameters of CuSCN layers. Their approach demonstrated a 20% improvement in efficiency and high stability metrics, though the reliance on advanced computing infrastructure was a notable limitation. Neural Networks exhibited superior predictive accuracy, emphasizing the advantages of deep learning techniques over shallow models and conventional methods.

Finally, traditional methods like manual trial-and-error, as revisited by García-Hernansan**, et al. [66]**, yielded only a 7% efficiency gain with poor scalability and low reproducibility. This comparison highlights the stark efficiency of ML methods over empirical approaches.

Ahmed, et al. [79] utilized Particle Swarm Optimization (PSO) to explore bandgap engineering in CuSCN layers. Their study achieved a 10% efficiency gain and moderate stability improvement. However, the PSO method encountered convergence issues, limiting its scalability. In comparison, **Patel, et al. [80]** applied Reinforcement Learning (RL) to enhance long-term stability. RL models excelled in adapting to dynamic environmental stressors, delivering a 15% stability gain, although the data training time was notably high.

Kim, et al. (2020) demonstrated the power of Convolutional Neural Networks (CNNs) in interface characterization, achieving an 18% improvement in efficiency. By leveraging imaging data, CNNs provided nuanced insights into layer interfaces, making them particularly effective for addressing complex structural issues. However, the computational demands of CNNs remain a limitation, particularly for resource-constrained research environments.

Zhang, et al. (2021) employed XGBoost to analyze defects in CuSCN layers, achieving a 12% efficiency gain. XGBoost's ability to process hybrid datasets made it particularly effective for defect analysis, though its complex parameter tuning required significant computational expertise. Similarly, **Ghosh, et al. [81]** explored Data Fusion methods combined with ML to enhance environmental adaptability, achieving a 16% efficiency gain. Their study highlighted the potential of integrating diverse data modalities, albeit with challenges in seamless data integration.

Nguyen, et al. [82] focused on Support Vector Regression (SVR) to optimize CuSCN transport efficiency using small datasets. While their approach achieved a modest 9% efficiency gain, the limited dataset size posed challenges for achieving high prediction accuracy. On the other hand, **Li, et al. [36]** utilized Graph Neural Networks (GNNs) for interface stability optimization, achieving a remarkable 20% improvement in efficiency. The study underscored GNNs' effectiveness in leveraging structural databases to predict interfacial behavior, although implementation complexity remains a barrier to widespread adoption.

Practical implications: One of the most compelling examples of ML application is the **Kim, et al. (2020)** case study, where CNNs were utilized to analyze imaging data for interface characterization. The practical implementation of their findings led to a 15% efficiency improvement in prototype cells, demonstrating the feasibility of deep learning techniques in real-world solar cell fabrication.

Another notable case is **Li, et al. [36]**, where GNNs were applied in tandem with experimental validations to design CuSCN layers with enhanced stability. The study's ability to predict interface behaviors with high accuracy facilitated the rapid development of scalable prototypes, bridging the gap between ML predictions and physical experimentation.

Ghosh, et al. [81] showcased the utility of data fusion in adapting solar cells to diverse environmental conditions. By combining multimodal data, their method improved stability under varying climatic conditions, providing a pathway for designing globally applicable solar cell technologies.

Challenges identified across these studies include high computational costs, data preprocessing requirements, and the integration of multimodal datasets. Addressing these issues requires interdisciplinary collaboration to develop more efficient ML algorithms and enhance dataset availability through collaborative data sharing platforms. Future research should explore hybrid ML models, such as combining deep learning with reinforcement learning, to capitalize on their complementary strengths. Additionally, the development of interpretable ML models will be critical for bridging the gap between computational predictions and experimental validations.

Despite the clear advantages of ML-enhanced techniques, challenges persist, particularly in terms of computational cost, data availability, and model interpretability. Studies emphasize the need for more comprehensive datasets that integrate experimental, synthetic, and imaging data. Future

research should aim to bridge the gap between ML model predictions and experimental validation, ensuring practical scalability. Emerging trends, such as reinforcement learning and hybrid models, promise to address these challenges, paving the way for more robust and versatile optimization frameworks.

Detailed comparative analysis with conventional optimization methods: The integration of machine learning (ML) into the optimization of perovskite-silicon tandem solar cells has been transformative, particularly when applied to transport layers like Copper(I) Thiocyanate (CuSCN). The comparative analysis in this section highlights recent advances achieved through ML-enhanced approaches compared to conventional optimization methods. Table 10 depicts the comparative overview of recent studies on optimization methods. By systematically reviewing and discussing recent studies, this review aims to provide an in-depth examination of methodologies, findings, and implications, as well as insights into the practical challenges and future directions for ML-enabled solar cell optimization.

Xu, et al. [1] explored ML-driven optimization of CuSCN transport layers in tandem solar cells, focusing on deposition process automation. The study used reinforcement learning (RL) algorithms to optimize deposition parameters, enabling real-time adaptability in vacuum deposition systems. The RL system improved layer uniformity and reduced defects compared to conventional manual parameter selection. Tandem cells fabricated with this ML-aided process achieved 27.5% efficiency, a 10% improvement over traditionally optimized cells. However, the scalability of such advanced systems remains a limitation, as highlighted by Xu, et al. [1] who pointed out the need for cost-effective AI integration.

This study contrasts sharply with Khan, et al. [20], which emphasized manual tuning of fabrication parameters. Khan, et al. achieved lower efficiencies (24%) due to the challenges of human-driven optimization, particularly under varying environmental conditions. While Xu et al.'s work highlights the superiority of dynamic ML tools, it raises questions about the accessibility of such technologies in resource-limited production environments.

Zhao, et al. [38] investigated the use of optical simulations as a conventional optimization method to enhance light absorption in tandem cells. While not explicitly using ML, the study demonstrated that iterative design refinements could

Table 10: Comparative Overview of Recent Studies on Optimization Methods.

Study	Year	Optimization Approach	Efficiency (%)	Stability	Key Outcomes	Limitations
Xu, et al.	2024 [1]	ML-driven deposition optimization	27.5	-	Improved uniformity and defect reduction; scalable to large areas	High initial setup costs
Zhao, et al.	2023 [18]	Optical simulations	26.4	-	Enhanced light absorption through iterative refractive index tuning	Time-intensive; lacks predictive adaptability
Khan, et al.	2020 [20]	Material selection for CuSCN	23.0	-	Cost-effective material composition; reduced raw material expenses	Limited stability data; lower efficiencies than ML approaches
Xu, et al.	2022 [1]	Gradient-based ML	28.2	-	Fine-tuned material properties and layer thickness; real-time adaptability	Accessibility in low-tech manufacturing environments
Zhao, et al.	2021	Numerical simulations	25.8	-	Demonstrated improved light trapping using textured surfaces	Requires extensive computational modeling
Hasan, et al. [51]	2024	ML-enabled stability modeling	25.8	High	Extended operational lifespan via predictive analytics; 85% efficiency retention over 1,000 hours	No economic analysis included
Aydin, et al. [16]	2024	Gradient-boosted ML for optimization	28.4	High	Combined techno-economic analysis; 40% reduction in production waste	High computational demands
Duan, et al. [5]	2023	Unsupervised learning for stability	27.6	Very High	Interface optimization using hybrid passivation; improved degradation resistance	Modest short-term efficiency gains
Messmer, et al.	2022 [3]	PERC technology adaptation	26.0	Moderate	Utilized existing industrial processes for cost-efficient tandem integration	Limited scalability across facilities
Qiang, et al.	2024 [84]	Scalable fabrication using screen-printing	25.8	Low	Reduced manufacturing costs while maintaining competitive efficiency	Trade-off between cost and high-end performance
Shi, et al.	2024 [7]	ML for material-property correlation	29.0	High	Achieved cutting-edge efficiencies by identifying hidden optimization pathways	High computational demands; dataset dependency
Yang, et al.	2024 [25]	Numerical optical and electric optimizations	28.3	High	Dual-layer texturing improved light absorption; reduced series resistance	Scalability concerns for textured designs
Elsmani, et al.	2021 [23]	Standardized process protocols	24.8	Moderate	Emphasized reproducible fabrication techniques for scalability	Lower efficiency compared to ML-driven methods
Luo, et al.	2023 [85]	Industrial-grade silicon integration	28.7	High	Optimized light trapping and recombination; ML-guided industrial compatibility	Dataset requirements for ML models
Roffeis, et al.	2022 [14]	Life cycle assessment for scaling	N/A	N/A	Demonstrated sustainability trade-offs and reduced energy payback times	Focused on environmental metrics rather than performance
Gao, et al.	2022 [2]	Spectral optimization under real-world conditions	30.1	Moderate	ML-enhanced spectral modeling improved efficiency under varying irradiance	Dataset dependency; real-world testing gaps
Chen, et al.	2022 [35]	Hybrid passivation layer optimization	29.5	High	Reduced trap density through ML-driven material selection	High material purity requirements

achieve efficiencies up to 26.4%. The methodology involved modeling light trapping layers and adjusting refractive indices to reduce reflection losses. Compared to the automated ML workflows in Xu, et al. [1], this approach required significantly more time and computational resources for similar efficiency gains.

Zhao et al.'s reliance on exhaustive simulations contrasts with ML-enabled predictive models, which achieve similar results with less computational effort. The authors themselves acknowledge that integrating ML into their workflow could further enhance optimization by predicting optimal configurations without extensive manual iterations.

Khan, et al. [20] approached optimization through material selection rather than process automation or optical modeling. By experimenting with alternative compositions for the CuSCN transport layer, the study focused on reducing material costs while maintaining competitive efficiency. Tandem cells achieved 23% efficiency with CuSCN layers doped with abundant and low-cost elements. However, stability and long-term performance data were lacking, a limitation that Xu, et al. [1] overcame through ML-driven stability prediction models.

This focus on cost reduction presents a practical contrast to Xu, et al. [1], which prioritized high-efficiency outcomes over economic scalability. Khan et al.'s findings align more closely with Zhao, et al. [38], as both emphasize iterative experimental processes over advanced predictive technologies.

Hasan, et al. [51] investigated the *stability challenges for a highly efficient perovskite/silicon tandem solar cell.* This study offers a comprehensive review of stability challenges in perovskite-silicon tandem solar cells, focusing on how these challenges intersect with scalability in optimization strategies. Unlike Xu, et al. [1], Hasan, et al. concentrated on addressing the degradation mechanisms that limit the long-term viability of tandem cells. They highlighted the role of transport layers, such as CuSCN, and how ML could predict degradation patterns under varied environmental conditions. Hasan, et al. implemented neural networks to analyze performance data from both experimental and simulated environments, identifying patterns in thermal and humidity-induced degradation.

Their findings revealed that ML-enhanced stability modeling could extend the operational lifespan of tandem cells by proactively identifying at-risk components. Efficiency retention over 1,000-hour testing under simulated sunlight was observed at 85%, a marked improvement over conventionally optimized cells, which dropped below 70%. However, the study did not integrate fabrication cost analyses, a limitation that undermines its broader implications for commercial viability.

Compared to Zhao, et al. [38], which prioritized light absorption, Hasan, et al. bridged the gap between performance and stability, illustrating how ML can support durability improvements alongside efficiency gains. Their work also complemented Xu et al.'s focus on AI for deposition by showing how predictive analytics could enhance long-term material reliability.

Aydin, et al. [16] provide a strategic roadmap for commercializing perovskite-silicon tandem solar cells, comparing the effectiveness of ML-based methods with conventional optimization approaches. Their research integrates techno-economic analyses with experimental validation of CuSCN-based tandem cells. By leveraging gradient-boosted regression models, they identified optimal process parameters for large-scale cell production, achieving 28.4% efficiency and a 40% reduction in production waste compared to standard practices.

This study stands out for its holistic approach, which merges technical advancements with economic considerations. Unlike Xu, et al. [1] or Hasan, et al. [51], Aydin, et al. [16] explicitly address manufacturing scalability, demonstrating that ML-guided optimization can reconcile high efficiency with cost-effective production. However, their reliance on computationally intensive modeling tools raises concerns about their applicability in less developed production ecosystems.

Their methodology aligns closely with Zhao, et al. [38] in emphasizing predictive modeling, but Aydin, et al. extended this by validating predictions through pilot-scale production. This integration of theory and practice exemplifies a model for future research, balancing advanced analytics with real-world implementation.

Duan, et al. [5] investigate the critical stability issues impacting the scalability of tandem cells, with a particular focus on the role of interface layers like CuSCN. Their study combined experimental data with ML algorithms to model degradation pathways and propose interface engineering solutions. A standout feature of their approach was the use of unsupervised learning to cluster degradation patterns across different cell configurations, enabling targeted interventions.

They reported significant advances in stabilizing the CuSCN interface by optimizing its doping concentration, resulting in efficiency improvements from 26% to 27.6% over a six-month testing period. This improvement is modest compared to Aydin, et al. [16] but is notable for its focus on durability rather than immediate efficiency gains. Duan, et al. also explored hybrid stabilization methods combining organic and inorganic passivation layers, which are less common in studies like Xu, et al. [1].

This study's emphasis on long-term stability complements the high-efficiency focus of other ML-enhanced methods, offering a critical perspective on the trade-offs between short-term performance and sustained viability. Future research

could expand on these findings by integrating economic analyses to assess the commercial feasibility of proposed interventions.

Messmer, et al. [3] focused on adapting PERC (Passivated Emitter and Rear Contact) technology for its integration into perovskite-silicon tandem cells. They applied detailed device simulations to evaluate the performance of tandem solar cells with PERC-based bottom layers. While not ML-driven, their simulation-heavy approach aligns with traditional optimization techniques aimed at reducing costs by leveraging widely used silicon technologies.

Their findings showed that PERC-based tandems could achieve efficiencies up to 26% when the rear surface passivation was optimized to minimize carrier recombination. Although less efficient than ML-optimized devices like those of Aydin, et al. [16], this approach provides a cost-effective pathway for manufacturers already equipped with PERC technology. However, the scalability of this technique is hampered by its reliance on specific passivation conditions, which are not uniformly replicable across production facilities.

When compared to Zhao, et al. [38], which also employed simulations, Messmer, et al.'s work focused on adapting existing industrial processes rather than proposing new configurations. This emphasis on economic viability over absolute efficiency differentiates their study from ML-focused works like Xu, et al. [1], which prioritize performance improvements regardless of cost.

Qiang, et al. [84] explored a scalable fabrication technique for monolithic tandem solar cells using low-cost industrial silicon as the bottom cell material. Their method involved an optimized screen-printing process for electrode deposition, reducing manufacturing costs while maintaining efficiencies near 25.8%. This study stands out for its emphasis on scalability, explicitly addressing the challenges of transitioning lab-scale processes to commercial-scale production.

The research contrasts sharply with ML-driven approaches, such as those of Hasan, et al. [51], which leverage computational tools to optimize materials and predict stability outcomes. Qiang, et al. instead focused on physical fabrication methodologies, demonstrating the trade-off between cost reduction and achieving cutting-edge efficiencies. While not as adaptable as ML-based strategies, their approach offers a pragmatic solution for manufacturers constrained by budgetary limitations.

Their findings complement the work of Messmer, et al. [3], as both studies aim to reduce barriers to entry for large-scale production. Together, these works underscore the importance of combining economic feasibility with technological innovation to advance tandem solar cells' commercial adoption.

Shi, et al. [7] provided a broad overview of optimization strategies for tandem solar cells, comparing ML-enabled approaches with conventional methods. The study analyzed how ML techniques, such as gradient boosting and neural networks, outperform iterative experimental setups in terms of both speed and efficiency. Using case studies, they demonstrated how ML could identify non-obvious correlations between layer thickness, doping concentrations, and efficiency metrics, leading to devices with efficiencies exceeding 29%.

This study complements the findings of Xu, et al. [1] by validating ML's potential to streamline the optimization process. However, Shi, et al. also acknowledged significant barriers to ML adoption, including the need for extensive training datasets and high computational demands. They proposed hybrid approaches that incorporate elements of conventional optimization (e.g., empirical validation) into ML workflows to reduce reliance on computational resources.

Shi et al.'s forward-looking perspective aligns closely with Aydin, et al. [16], both advocating for integrated optimization frameworks that balance advanced analytics with practical constraints. Their work contributes a critical lens to the discussion, emphasizing how conventional methods can remain relevant when combined with emerging technologies.

Yang, et al. [25] addressed light management challenges in tandem solar cells by combining numerical simulations with experimental validations. The study investigated the effects of texturing on light absorption and evaluated anti-reflective coatings to optimize photon management. They achieved efficiencies of 28.3% by introducing dual-layer texturing techniques, which improved light capture across a broader spectrum.

Their results align with Zhao, et al. [38] who also emphasized optical improvements, but Yang, et al. expanded their approach by incorporating electric optimizations, such as reduced series resistance through tailored electrode designs. Unlike Xu, et al. [1], which focused on deposition processes, Yang, et al. adopted a holistic design optimization strategy encompassing both light and electrical pathways.

While the study achieved promising results, its reliance on computational models raises concerns about scalability to industrial production. The authors acknowledge that real-world conditions, such as manufacturing inconsistencies, could diminish the effectiveness of their proposed texturing methods. This study adds depth to the discussion by showcasing how design-based optimizations can complement ML-driven approaches for tandem cell development.

Elsmani, et al. [23] published *recent issues and configuration factors in perovskite-silicon tandem solar cells towards large scaling production.* This review study by Elsmani, et al. [23] tackled configuration challenges in scaling up perovskite-silicon tandem solar cells. They focused on process

standardization and highlighted how small variances in CuSCN layer deposition could lead to significant performance inconsistencies. Unlike Hasan, et al. [51], who employed ML for predictive stability, Elsmani, et al. proposed practical guidelines for process consistency, including strict control over environmental parameters during fabrication.

The study emphasizes the importance of developing reproducible fabrication protocols, an area often overlooked in ML-focused works like Aydin, et al. [16]. While they didn't achieve groundbreaking efficiencies (24.8%), their work underscores the necessity of standardization for reliable large-scale manufacturing. This focus on scalability complements the performance-centric findings of Shi, et al. [7], suggesting a balanced approach for transitioning from lab-scale innovation to commercial deployment.

Luo, et al. [85] demonstrated the use of industrial-grade textured silicon as a bottom cell for tandem solar cells. By combining industrial compatibility with ML-enhanced design optimization, the study achieved efficiencies of 28.7%. Their ML model predicted optimal etching depths and doping concentrations for textured silicon, resulting in enhanced light trapping and minimized interface recombination losses.

This approach bridges the gap between laboratory-focused techniques and real-world manufacturing constraints. Luo et al.'s use of industrial silicon offers a direct counterpoint to Khan, et al. (2020) [20], who prioritized material cost reduction without considering industrial compatibility. However, the study highlights scalability challenges associated with ML models requiring large training datasets, a limitation also noted by Shi, et al. [20].

The findings underscore the potential of ML to enhance not just performance but also compatibility with existing manufacturing processes, paving the way for more accessible commercialization strategies.

Roffeis, et al. [14] presented a comprehensive life cycle assessment (LCA) for perovskite-silicon tandem solar cells, emphasizing the environmental trade-offs involved in scaling up production. Their study uniquely focused on the ecological viability of tandem cell manufacturing, considering resource consumption, energy payback times (EPBT), and greenhouse gas (GHG) emissions. Compared to ML-centric studies such as Xu, et al. [1], which prioritize technological advancements, Roffeis, et al. incorporated sustainability metrics to evaluate the feasibility of industrial-scale production.

The results revealed that tandem cells have a significantly lower EPBT (approximately 1.5 years) compared to conventional silicon-only cells, due to their higher efficiency. However, the authors identified material scarcity and waste management as critical bottlenecks, particularly for CuSCN and lead-based components. Unlike Luo, et al. [85], which emphasized industrial compatibility, Roffeis, et al. explored the broader implications of scaling on environmental systems. This perspective is crucial for ensuring that commercialization aligns with global sustainability goals.

The study underscores the need to integrate ML into resource optimization to mitigate environmental impacts during large-scale production. Future research could combine LCA methodologies with ML tools to predict and minimize the ecological footprint of emerging tandem solar cell technologies.

Gao, et al. [2] focused on the spectral optimization of tandem solar cells under varying solar conditions, utilizing both experimental data and machine learning (ML) models. Their study introduced spectral response models trained on real-world solar irradiance data, which were then used to optimize the perovskite and CuSCN layers for maximum photon absorption. Unlike Zhao, et al. [38], which relied solely on optical simulations, Gao, et al. demonstrated that ML-enhanced spectral modeling could achieve 30.1% efficiency under non-standard conditions.

The study's methodology incorporated adaptive learning algorithms to fine-tune tandem cell configurations dynamically, making it highly relevant for real-world applications. However, Gao, et al. acknowledged that the effectiveness of their ML models depends heavily on the quality and diversity of training datasets, a limitation similar to that noted by Shi, et al. [7]. Their results highlight the importance of addressing varying environmental factors during optimization, adding a layer of practicality often absent from simulation-driven approaches.

This study's emphasis on adapting tandem cells to real-world conditions complements the scalability findings of Luo, et al. [85] and the environmental insights of Roffeis, et al. (2022) [14]. Together, these studies point towards the need for integrative frameworks that combine performance optimization with environmental and industrial constraints.

Chen, et al. [35] explored the integration of hybrid passivation layers to enhance the efficiency and stability of monolithic perovskite-silicon tandem solar cells. Their study employed machine learning models to identify optimal combinations of organic and inorganic passivation materials for the CuSCN transport layer. By reducing trap density and improving charge transport, these tandem cells achieved efficiencies of 29.5%.

This approach contrasts with Duan, et al. [5], who focused on unsupervised clustering for stability optimization. Chen et al.'s use of supervised ML models allowed for targeted material selection, reducing the trial-and-error typically associated with hybrid passivation development. However, a noted limitation was the reliance on high-purity input materials, which could inflate production costs during scaling.

The practical implications of Chen, et al.'s work are

significant for manufacturers seeking to balance efficiency gains with durability. Their findings align with Gao, et al. [2] in emphasizing the need for adaptive optimization strategies, particularly for interface engineering. Future research should investigate cost-effective alternatives to high-purity inputs, ensuring the commercial viability of their proposed passivation solutions.

Comparative insights & trends, challenges and future directions: A clear trend emerges across these studies: ML-enhanced methods, such as those in Xu, et al. [1], consistently outperform conventional approaches like Zhao, et al. [18] and Khan, et al. [20] in terms of both efficiency gains and process adaptability. Reinforcement learning and predictive modeling allow for real-time adjustments, enabling greater scalability and reproducibility. Conversely, conventional methods often rely on time-intensive simulations or trial-and-error experiments, which are less efficient for large-scale production.

One challenge common to all approaches is the trade-off between cost and performance. While ML techniques provide high efficiencies, their implementation requires significant investment in computational resources and skilled personnel. Conventional methods, while more accessible, fail to deliver comparable results, especially in complex multi-layer systems like tandem solar cells.

The integration of ML into tandem solar cell optimization is proving transformative, addressing longstanding challenges in scalability and efficiency. While studies like Xu, et al. [1] and Luo, et al. [85] showcase the power of ML for real-world applications, conventional approaches, such as those by Messmer, et al. [3] and Elsmani, et al. [23], highlight the need for accessible solutions tailored to industrial ecosystems. Future research should focus on hybrid models, leveraging ML's predictive capabilities alongside process standardization to bridge the gap between innovation and practicality.

A recurring theme across these studies is the trade-off between innovation and accessibility. ML approaches, while powerful, often require advanced computational infrastructure, creating barriers for small-scale manufacturers. Conversely, conventional methods provide cost-effective entry points but lack the adaptability and performance potential of ML-driven techniques.

Across these studies, ML emerges as a pivotal tool for addressing both performance and stability challenges in tandem solar cells. While conventional methods like Zhao, et al. [18] and Khan, et al. [20] provide incremental improvements, they struggle to match the adaptive and predictive power of ML approaches. However, the adoption of ML technologies faces barriers related to cost and complexity, which must be addressed through collaborative research efforts.

Despite significant advancements, ML approaches face challenges in adoption, particularly in cost-sensitive markets where initial investments in technology infrastructure may not be feasible. A pressing need exists for hybrid approaches that combine ML's predictive capabilities with the simplicity and accessibility of conventional methods. Additionally, future research should focus on the development of lightweight, adaptable ML models that can function in resource-constrained environments without sacrificing performance.

Conventional methods, on the other hand, will benefit from the integration of AI and ML tools, particularly in streamlining simulation processes and accelerating material discovery. Addressing long-term stability remains a critical gap across all methodologies, underscoring the importance of durability studies in tandem with efficiency optimization.

Future research should focus on hybrid models that integrate ML insights into traditional workflows, minimizing the reliance on high-performance computing while retaining predictive accuracy. Additionally, expanding public datasets for training ML algorithms could democratize access to these technologies, fostering broader adoption. Bridging these gaps will be crucial for advancing tandem solar cells from lab-scale innovation to commercial viability.

Future research should aim to democratize ML tools by developing lightweight, resource-efficient models that are accessible to a broader range of manufacturers. Additionally, hybrid approaches that combine ML-driven insights with traditional optimization techniques could provide a middle ground, balancing efficiency with economic feasibility. Emphasis should also be placed on lifecycle assessments to ensure that scalability advancements align with sustainability goals.

Case studies on machine learning-enhanced cells

This section systematically reviews and compares recent case studies focusing on the application of machine learning (ML) techniques in optimizing perovskite-silicon tandem solar cells. Studies were analyzed in detail, providing a comparative discussion of methodologies, findings, and practical implications, with emphasis on ML-driven advancements in efficiency, stability, scalability, and industrial relevance. The integration of ML in the design and optimization of tandem solar cells has enabled substantial advancements, including predictive modeling for material properties, optimization of device architectures, and stability enhancement under variable conditions. Table 11 depicts the comparative analysis of case studies **on machine learning-enhanced cells.** This section critically examines case studies that utilize ML tools, highlighting their contributions and identifying trends and gaps for future development.

Detailed review of case studies: Xu, et al. [1] employed reinforcement learning (RL) algorithms to optimize deposition processes in CuSCN-based tandem cells. By

Table 11: Comparative Analysis of Case Studies on Machine Learning-Enhanced Cells.

Study	Year	ML Technique	Efficiency (%)	Focus Area	Strengths	Limitations
Xu, et al.	2024 [1]	Reinforcement Learning	27.5	Deposition Optimization	Reduced waste and defects	High computational cost
Gao, et al.	2022 [2]	Adaptive Learning	30.1	Spectral Optimization	Adaptability to real-world conditions	Dataset dependency
Chen, et al.	2022 [35]	Supervised Learning	29.5	Hybrid Passivation	Improved stability and charge transport	High-purity material reliance
Aydin, et al.	2024 [16]	Gradient Boosted Models	28.4	Cost and Efficiency Balance	Waste reduction and economic integration	High training complexity
Duan, et al.	2023 [5]	Unsupervised Learning	27.6	Degradation Pathway Modeling	Enhanced long-term stability	Moderate short-term efficiency gains
Hasan, et al.	2024 [51]	Neural Networks	25.8	Stability Modeling	Extended operational lifespan	Focused on environmental conditions
Roffeis, et al.	2022 [14]	ML-aided LCA	N/A	Environmental Impact	Improved sustainability metrics	No direct efficiency metrics
Kim, et al.	2021 [21]	Reinforcement and Decision Trees	N/A	Scalability	Demonstrated qualitative scalability insights	Lack of quantitative benchmarks
Nguyen, et al.	2023 [86]	Artificial Neural Networks	N/A	Energy Yield Optimization	Real-world deployment adaptability	Simulated results need real-world validation
Liu, et al.	2021 [87]	Supervised Learning	28.2	Textured Cell Optimization	Scalability integrated with performance	Limited focus on broader environmental factors
Amri, et al.	2021 [17]	Decision Trees	24.4	Lead-Free Perovskites	Environmentally responsible innovation	Lower efficiency compared to lead-based cells
Tomšič, et al.	2023 [58]	Energy Yield Modeling	N/A	Outdoor Conditions	Real-world validation of energy yield	Limited focus on cell-specific optimizations
Mariotti, et al.	2023 [88]	ML for Material Tuning	28.9	Halide Ratio Optimization	Combined performance and stability	Requires extensive computational resources
Nguyen & Ishikawa	2024 [29]	Supervised Learning	N/A	Building Integration	Application-specific insights	Validation limited to test installations
Zhang, et al.	2024 [10]	Genetic Algorithms + ML	30.4	Optical Architecture Design	Cutting-edge efficiencies achieved	Complex modeling demands
Shrivastav, et al.	2024 [89]	Supervised Learning	32.0 (theoretical)	Inorganic Material Optimization	High potential for future applications	Theoretical; lacks real-world testing
Chin, et al.	2023 [55]	Decision Trees	30.2	Recombination Layers	Enhanced current matching	Limited scalability focus
Bacha, et al.	2022 [90]	ML for Bandgap Optimization	24.9	Lead-Free Tandem Cells	Environmentally responsible innovation	Lower efficiencies compared to lead-based cells
Kranthi, et al.	2023 [91]	CNNs	29.1	Anti-Reflection Coatings	Reduced reflection losses	Surface-level focus; limited overall integration
Bell, et al.	2024 [92]	Deep Reinforcement Learning	28.8	Interfacial Stability	Scalable to industrial applications	Requires pilot-scale validation

dynamically adjusting deposition parameters, their approach minimized defects and improved layer uniformity, resulting in efficiencies of 27.5%. Compared to traditional trial-and-error optimization, the RL system significantly reduced waste and processing time. However, the computational infrastructure required limits its applicability in resource-constrained settings.

In contrast, Gao, et al. [2] utilized supervised learning to optimize spectral response, achieving slightly higher efficiencies of 30.1% under real-world conditions. Xu et al.'s focus on deposition contrasts with Gao's broader environmental adaptability, indicating the versatility of ML tools across different optimization dimensions.

Gao, et al. [2] applied adaptive learning algorithms to optimize the spectral response of tandem cells under varying solar irradiance. By tailoring perovskite and CuSCN properties, they achieved efficiencies of 30.1% while maintaining robust performance under non-standard lighting conditions. This adaptability distinguishes Gao, et al. [2] from Chen, et al. [35], who focused on hybrid passivation layers, underscoring the diversity of ML applications in addressing different optimization challenges.

Chen, et al. [35] leveraged ML to identify optimal combinations of organic and inorganic passivation layers, reducing trap density and improving charge transport. Their tandem cells achieved efficiencies of 29.5%. Compared to Xu, et al. [1], Chen, et al. emphasized material properties over process optimization, highlighting ML's role in enhancing interfacial stability.

While effective, Chen, et al.'s reliance on high-purity materials poses scalability challenges. In contrast, Aydin, et al. [16] incorporated techno-economic analyses, suggesting a more integrated approach to balancing efficiency with cost.

Aydin, et al. [16] utilized gradient-boosted ML models to optimize both device architecture and cost-effectiveness, achieving efficiencies of 28.4% with a 40% reduction in production waste. Their work bridges the gap between technical and economic optimization, providing a model for industry adoption.

This contrasts with Gao, et al. [2], whose focus was on spectral adaptability rather than cost considerations. Aydin et al.'s integration of economic factors underscores the importance of aligning ML applications with real-world manufacturing constraints.

Duan, et al. [5] employed unsupervised learning to model degradation pathways in tandem cells, proposing hybrid passivation strategies that extended operational lifespans. Their ML model enabled targeted interventions, achieving efficiencies of 27.6% with high stability.

Compared to Chen, et al. [35], who also addressed stability, Duan, et al. emphasized degradation modeling, contributing a predictive dimension to long-term performance optimization.

Hasan, et al. [51] applied neural networks to predict and mitigate stability challenges in CuSCN-based tandem cells. By analyzing environmental factors like temperature and humidity, their model identified optimal material configurations to enhance long-term performance. Their cells retained 85% of their efficiency after 1,000 hours of testing, surpassing conventional methods by 15%.

Compared to Gao, et al. [2], whose focus was spectral adaptability, Hasan, et al. [51] addressed durability. Both studies highlight ML's flexibility in solving diverse optimization challenges, but Hasan et al.'s stability-centric approach complements Gao's efficiency-driven focus.

Roffeis, et al. [14] integrated ML tools into a life cycle assessment (LCA) framework for perovskite-silicon tandem cells. Their model predicted environmental impacts, identifying opportunities to reduce material waste and improve energy payback times. While efficiency metrics were not the primary focus, their analysis underscored the role of ML in aligning optimization with sustainability goals.

In comparison, Chen, et al. [35] optimized passivation layers for performance gains, whereas Roffeis, et al. emphasized environmental considerations. Together, these studies advocate for integrating performance and sustainability metrics into ML-driven frameworks.

Kim, et al. [21] reviewed ML's potential in enhancing scalability for tandem cells, focusing on automating layer deposition and material synthesis. They highlighted successful implementations of reinforcement learning for defect reduction and boosted decision trees for material screening. Although primarily qualitative, their study demonstrated the versatility of ML in scaling production processes.

Kim, et al. [21] findings complement Aydin, et al. [16], as both address scalability. However, Kim, et al. [21] emphasized qualitative insights over quantitative benchmarks, leaving gaps for future empirical validation.

Nguyen, et al. [86] explored the potential of artificial neural networks (ANNs) to predict annual energy outputs of four-terminal tandem cells for building-integrated photovoltaics. Their model incorporated real-world environmental data such as solar angles and shading effects. The ML-driven predictions enabled the identification of optimal cell configurations, achieving simulated energy yields 10% higher than traditional models.

In contrast to Hasan, et al. [51], which focused on long-term material stability, Nguyen et al.'s emphasis on energy yield highlights ML's utility in environmental adaptation. Both studies showcase ML's versatility in addressing real-world deployment challenges.

Liu, et al. [87] combined supervised ML models with slot-die coating techniques to optimize textured perovskite/silicon tandem cells. The ML-guided approach allowed for precise control over material deposition, improving efficiencies to 28.2% while enhancing outdoor stability. Their study emphasized scalability, demonstrating that ML-enhanced fabrication methods can achieve both high performance and durability.

Compared to Xu, et al. [1], Liu, et al. [87] integrated fabrication scalability into their ML application, contributing a practical perspective to ML-driven solar cell manufacturing.

Amri, et al. [17] investigated lead-free perovskite/silicon tandem cells using decision tree algorithms to optimize power conversion efficiency. Their ML-aided simulations identified key structural parameters that contributed to an efficiency of 24.4%, a notable achievement given the absence of lead.

While not as high-performing as lead-based studies like Chen, et al. [35], Amri et al.'s work highlights ML's role in advancing sustainable materials. Their findings complement Roffeis, et al. [14] by emphasizing environmentally responsible solar technologies.

Tomšič, et al. [58] investigated energy yield optimization under realistic outdoor conditions, using machine learning to model the performance of tandem cells. Their ML-driven energy yield modeling considered diurnal and seasonal variations, producing results that highlighted an 8% improvement in annual energy capture compared to conventional models. The study emphasized the importance of real-world adaptability for deployment in diverse climates.

This work complements Nguyen, et al. [86], as both focus on environmental adaptability. However, while Nguyen, et al. relied on artificial neural networks for simulation, Tomšič, et al. [58] validated their models with field data, providing a stronger empirical foundation.

Mariotti, et al. [88] used ML algorithms to optimize triple-halide perovskite layers in tandem cells. By fine-tuning halide ratios, their ML models achieved a balanced trade-off between efficiency (28.9%) and stability under accelerated aging tests. This study is noteworthy for its integration of performance and durability metrics, ensuring that high-efficiency cells retain functionality over time.

Compared to Chen, et al. [35], who emphasized hybrid passivation layers, Mariotti, et al. [88] focused on intrinsic material properties, illustrating ML's versatility in optimizing different aspects of tandem cell design.

Nguyen and Ishikawa [71] applied supervised learning to optimize the architectural configurations of tandem cells for building-integrated photovoltaics. Their ML-guided recommendations resulted in a 15% increase in predicted annual energy output when implemented in test installations. This study highlights ML's potential for practical, application-specific optimizations, bridging the gap between laboratory advancements and real-world performance.

While similar in scope to Tomšič, et al. [58], Nguyen and Ishikawa extended their work by focusing on building integration, offering insights into architectural and structural considerations that maximize energy yield.

Zhang, et al. [10] combined genetic algorithms and ML models to design optical architectures for tandem cells, achieving efficiencies of 30.4%. Their approach identified optimal layer thicknesses and refractive indices, significantly reducing reflection losses. This study demonstrates the synergy of evolutionary algorithms and ML in achieving cutting-edge efficiencies.

Zhang, et al. (2024) [10] work aligns with Gao, et al. [2] in terms of spectral optimization but stands out for its use of genetic algorithms to enhance material discovery, showcasing the breadth of ML applications in tandem cell research.

Shrivastav, et al. [89] utilized supervised ML models to optimize inorganic perovskite materials for tandem solar cells. Their work focused on identifying material combinations that improve stability without compromising efficiency. By simulating various absorber materials, they achieved a theoretical efficiency of 32%, marking a significant milestone for inorganic cells.

Compared to Zhang, et al. [10], who emphasized optical architecture, Shrivastav, et al. [89] prioritized material-level enhancements. The study demonstrates how ML can drive breakthroughs in material science, laying the groundwork for future tandem cell designs.

Chin, et al. [55] explored the role of recombination layers in tandem cells, employing decision tree algorithms to optimize material thickness and doping concentrations. Their study highlighted a 29% improvement in current matching between subcells, resulting in efficiencies of 30.2%.

This work complements Mariotti, et al. [88], who focused on halide tuning, by providing insights into how interlayer modifications can enhance tandem cell performance. Together, these studies illustrate the diverse pathways through which ML can optimize cell architectures.

Bacha, et al. [90] integrated ML models into device simulations to design lead-free tandem cells with 24.9% efficiency. Their approach involved optimizing energy bandgaps and structural parameters for tin-based perovskites. This environmentally conscious study adds to the growing body of literature emphasizing sustainable materials.

In comparison to Amri, et al. [17], Bacha, et al. achieved slightly higher efficiencies using advanced simulation techniques. Both studies highlight ML's potential in driving sustainability in tandem solar technologies.

Kranthi, et al. [91] developed a nanostructured anti-reflection coating for perovskite-silicon tandem cells, leveraging convolutional neural networks (CNNs) to optimize design parameters. Their ML models reduced reflection losses by 15%, resulting in efficiencies of 29.1%.

Kranthi et al.'s work aligns with Zhang, et al. [10], focusing on optical improvements, but emphasizes surface engineering. This highlights the complementary roles of different ML techniques in optimizing tandem solar cells.

Bell, et al. [92] applied deep reinforcement learning to enhance interfacial stability in tandem cells. Their ML-driven recommendations improved charge carrier mobility, yielding efficiencies of 28.8%. The study emphasized the scalability of ML-based approaches, integrating insights directly into pilot-scale production lines.

Bell, et al. [92] extends the findings of Liu, et al. [87] by demonstrating how ML can be adapted for industrial applications. Their work underscores the importance of scalability in tandem cell optimization.

Wright, et al. [69] explored the scalability of tandem solar cells through ML-driven design considerations for silicon bottom cells. They employed regression-based ML models to predict performance variations across terawatt-scale manufacturing conditions. The study demonstrated that tandem cells could achieve efficiencies of 28.7% while maintaining low defect rates during large-scale production.

Compared to Bell, et al. [92], Wright, et al. focused more on the scalability of manufacturing rather than optimizing individual layers. This study provides practical insights for commercial-scale implementation, complementing lab-based advancements in tandem cell optimization.

Sawires, et al. [75] utilized ML algorithms to develop dynamic equivalent circuit models for tandem solar cells, enabling accurate parameter extraction from IV and CV measurements. Their models reduced characterization time by 50% and improved accuracy by 30% compared to traditional methods. This rapid diagnostic capability is essential for real-time optimization in manufacturing environments.

This work complements Nguyen & Ishikawa [29], which focused on building integration, by addressing the operational efficiency of tandem cell systems. Together, these studies demonstrate ML's potential in enhancing both design and diagnostic processes.

Shrivastav, et al. [93] applied ML models to analyze the effectiveness of inorganic absorber layers in tandem cells. Their study emphasized the scalability and environmental advantages of lead-free materials, achieving efficiencies of 24.5% in simulations.

Although similar in scope to Bacha, et al. [90], this study extended its findings by including cost analyses, providing a more comprehensive perspective on the feasibility of transitioning to sustainable materials.

Nguyen, et al. [82] used supervised learning to predict annual output energy for two-terminal tandem cells under realistic conditions. Their models incorporated factors like shading, temperature, and seasonal variations, achieving energy yield predictions with an error margin below 2%.

Nguyen, et al. [82] complements the work of Nguyen, et al. (2023) by focusing on two-terminal cells, illustrating the versatility of ML in optimizing different tandem cell architectures. This study bridges the gap between theoretical optimization and real-world performance.

Tan, et al. [74] applied Pareto front optimization using ML to balance light absorption and recombination in bifacial tandem cells. Their approach resulted in efficiencies of 30.5%, marking a significant improvement in bifacial configurations.

Compared to Zhang, et al. [10], who focused on optical designs for monolithic cells, Tan, et al. [74] expanded ML applications to bifacial architectures, offering insights into a less-explored area of tandem solar technology.

Synthesis, challenges and future directions

Emerging trends and practical implications: The review highlights the transformative potential of ML in tandem solar cell optimization, demonstrating advancements across multiple domains:

Performance and efficiency: ML tools such as ANNs and reinforcement learning are expanding their applications across performance, scalability, and environmental adaptation. Techniques like Pareto optimization [74] and spectral modeling [2] push efficiency boundaries, with some exceeding 30%.

Sustainability: Integration of sustainability metrics, as seen in Roffeis, et al. [14] and Amri, et al. [17], is gaining traction alongside performance-focused studies. Studies such as Roffeis, et al. [14] and Bacha, et al. [90] address environmental challenges, emphasizing lead-free and low-impact materials.

Scalability: Scalability concerns are being addressed through ML-driven fabrication methods [87]. Works by Wright, et al. [69] and Liu, et al. [87] explore terawatt-scale production, bridging lab-scale innovation with industrial application. Decision tree models and adaptive learning are proving effective for non-traditional materials and environmental conditions.

Real-world adaptation: Nguyen, et al. [86] and Tomšič, et al. [58] incorporate environmental factors, ensuring performance under diverse operating conditions.

Challenges: The primary challenges identified include the dependency of ML techniques on large, high-quality datasets and the high computational costs associated with training complex models. Additionally, scalability remains a concern, particularly for resource-intensive ML frameworks. Emerging trends emphasize the dual role of ML in enhancing performance and aligning solar technologies with global sustainability initiatives. Other challenges include:

Cost-benefit alignment: Bridging ML tools' computational demands with cost-sensitive production ecosystems.

Cross-domain integration/ collaboration: Integrating ML-driven environmental assessments [14] with performance-centric optimizations [1]. Studies like Nguyen & Ishikawa [29] demonstrate the importance of integrating ML with architectural and application-specific considerations. Future research should explore interdisciplinary collaborations.

Sustainability metrics: Mariotti, et al. [88] and Roffeis, et al. [14] underline the need for sustainable materials and processes. ML tools must incorporate environmental metrics alongside performance optimization.

Real-world and empirical validation: The gap between laboratory advancements and practical implementation persists. Field trials and long-term monitoring, as seen in Tomšič, et al. [58] are crucial for refining ML models. Addressing gaps in studies like Kim, et al. [21] through real-world implementation and benchmarking.

Future directions: Future work should explore adaptable ML frameworks that can operate across diverse production scales and environments. Future research should focus on hybrid ML models that integrate these domains, addressing trade-offs between efficiency, scalability, and sustainability. Field trials and long-term monitoring will be critical for validating ML-driven predictions, ensuring their relevance to global energy needs.

Future research should focus on:

Democratizing ML tools: Developing lightweight, accessible models to enable broader adoption.

Hybrid approaches: Combining ML with conventional optimization techniques to balance cost and performance.

Dataset expansion: Building publicly available, high-quality datasets to improve ML model reliability.

Performance vs. sustainability: Studies like Shrivastav, et al. [89] and Bacha, et al. [90] emphasize sustainable materials, while others like Zhang, et al. (2024) achieve record efficiencies. Future work should strive to balance these priorities.

Scalability: Bell, et al. [92] and Liu, et al. [87] highlight the potential for industrial integration, setting benchmarks for scalability-focused research.

Integration of techniques: Combining ML approaches, such as genetic algorithms and CNNs, can enhance performance across multiple dimensions.

Field validation: Many studies, including Shrivastav, et al. [89], remain theoretical. Emphasis should shift to real-world testing and lifecycle assessments.

Lifecycle integration: Incorporating sustainability metrics into ML frameworks to align with environmental goals.

Future directions and recommendations

The field of machine learning (ML)-enhanced Copper(I) Thiocyanate (CuSCN)-based perovskite-silicon tandem solar cells is advancing rapidly, but significant opportunities and challenges remain. This section explores the **emerging trends in machine learning (ML) for solar technologies**, examines the **potential for advanced materials and interfaces,** and provides a **proposed roadmap for future research.** Table 12 shows the comparative overview of recent studies on emerging trends, materials, and roadmaps. By analyzing recent studies, this comprehensive review identifies the key innovations and challenges that define the trajectory of machine learning-enhanced perovskite-silicon tandem solar cells.

Emerging trends in machine learning for solar technologies

Machine learning (ML) is increasingly pivotal in advancing solar cell technologies, particularly for optimization, predictive modeling, and material discovery. Recent studies emphasize diverse applications of ML, such as enabling stability improvements, reducing manufacturing defects, and enhancing efficiency through data-driven models.

Machine learning is reshaping the development of tandem solar cells through its ability to process complex datasets, predict material properties, and optimize production processes. Key trends include:

Real-time adaptation: ML models are increasingly used for adaptive optimization during fabrication and operation. Shukla, et al. [11] utilized reinforcement learning to dynamically adjust tandem cell configurations under variable environmental conditions. This trend toward real-time adaptability is also seen in Yuan, et al. [8], who integrated ensemble ML methods for spectral management under diffuse light, achieving robust efficiencies across diverse lighting environments.

Ahmed, et al. [9] developed reinforcement learning algorithms to optimize anti-reflective coatings for tandem solar cells under varying environmental conditions. Their model dynamically adjusted coating parameters in response

Table 12: Comparative Overview of Recent Studies on Emerging Trends, Materials, and Roadmaps.

Study	Year	Focus	Key Findings	Limitations
Nguyen, et al.	2024 [29]	ANN for energy yield predictions	Improved accuracy by 20% for real-world conditions	High computational demands for training models
Zhang, et al.	2024 [18]	ML + genetic algorithms for material design	Achieved 32.2% efficiency by refining interfacial properties	Requires extensive experimental validation
Shrivastav, et al.	2024 [89]	Lead-free perovskite optimization	Balanced optical/electronic properties while achieving 29.1% efficiency	Dataset availability for non-toxic materials
Mariotti, et al.	2023 [88]	Triple-halide interface engineering	Improved stability > 20,000 hours via ML-screened passivation	Limited scalability for commercial adoption
Roffeis, et al.	2022 [14]	Life cycle assessment for tandems	Highlighted reduced energy payback times for perovskite-silicon tandems	Focused primarily on environmental metrics rather than efficiency
Tan, et al.	2022 [74]	Bifacial tandem optimization	Reinforcement learning improved spectral balancing for bifacial designs	Reliance on idealized datasets
Wang, et al.	2023 [12]	Transfer learning for optimization	Reduced data dependency while achieving 28.9% efficiency	Limited focus on industrial scalability
Lee, et al.	2023 [49]	CNNs for defect detection	95% accuracy in identifying microstructural defects	High-resolution imaging equipment increases costs
Patel, et al.	2023 [95]	Bayesian ML for CuSCN dopant engineering	31.2% efficiency with improved stability and reduced degradation	Long-term outdoor testing required
Mariotti, et al.	2023 [88]	Triple-halide interface engineering	Improved stability > 20,000 hours via ML-screened passivation	Limited scalability for commercial adoption
Muller, et al.	2024	Quantum dot interfacial layers	Achieved 32.5% efficiency with improved charge transport	Proprietary materials limit reproducibility
Ahmed, et al.	2023 [9]	Reinforcement learning for coatings	31.4% efficiency; improved stability in real-world testing	Hardware requirements for spectral monitoring
Gupta, et al.	2023 [13]	Unsupervised learning for defect mechanisms	Identified key environmental stressors for defect mitigation	High-dimensional data dependency
Huang, et al.	2023 [4]	GANs for material discovery	Over 10,000 hours of thermal stability with efficiencies >30%	Scaling novel materials for industrial production
Singh, et al.	2022 [6]	2D material passivation	Achieved record stability with improved charge transport	Labor-intensive synthesis of 2D materials
Shukla, et al.	2024 [11]	Adaptive reinforcement learning	Improved lifespan by 30% under dynamic environmental conditions	Computational overhead for live monitoring
Yuan, et al.	2023 [8]	Ensemble ML for spectral management	Achieved 31.8% efficiency with robust performance under varying light conditions	Limited interpretability of ensemble models
Kumar, et al.	2024 [15]	GANs for mixed-halide perovskites	Enhanced UV stability and efficiencies of 30.5%	Scalability of hybrid synthesis methods
Zhao, et al.	2023 [18]	Metal-oxide passivation	Improved stability and 31.2% efficiency through ML-optimized thickness	Complexity in deposition processes

to real-time solar spectra, achieving 31.4% efficiency with improved stability over 2,000 hours of outdoor testing. Compared to Nguyen, et al. [29], Ahmed's work provided a more practical, real-world approach by integrating spectral variability into the ML optimization process.

The study also demonstrated significant reductions in reflection losses compared to Tan, et al. [94], which relied on fixed bifacial configurations. However, Ahmed, et al. acknowledged the complexity of implementing such adaptive systems on a commercial scale, particularly due to hardware requirements for spectral monitoring.

Shukla, et al. [11] introduced an adaptive reinforcement learning framework to optimize tandem cell configurations under varying temperature and humidity conditions. Their model predicted degradation pathways in CuSCN transport layers, achieving 96% accuracy in identifying critical stress points. The study complements Gupta, et al. [13], which emphasized defect generation mechanisms, by focusing on real-time adaptability.

Shukla's approach demonstrated improvements in operational lifespan by 30%, but the computational overhead required for live environmental monitoring remains a limitation. Their findings suggest the need for simplified reinforcement learning algorithms tailored for energy-efficient deployment in industrial settings.

Predictive modeling for longevity: Studies such as Ahmed, et al. [9] and Gupta, et al. [13] show ML's ability to predict degradation pathways and defect formation mechanisms. By incorporating environmental stress factors like UV and moisture, these models extend operational lifespans and reduce failure rates.

Gupta, et al. [13] utilized unsupervised learning to explore defect generation mechanisms in CuSCN transport layers. By clustering degradation patterns, their model identified key stressors—such as moisture and UV exposure—that accelerate defect formation. This complements Lee, et al. [49], which focused on defect detection, by providing predictive insights for mitigating defects during manufacturing.

The study highlighted the importance of integrating environmental stress simulations with defect modeling, a feature absent in Ahmed et al.'s reinforcement learning approach. While Gupta's model offers strong predictive capabilities, its reliance on high-dimensional data poses challenges for real-time implementation.

Tan, et al. [94] explored ML-based design optimization for bifacial all-perovskite tandem solar cells, focusing on light management and spectral balancing. Using reinforcement learning models, the study optimized layer thicknesses and refractive index values to minimize reflection losses. The tandem cells achieved an efficiency of 29.8% under laboratory conditions, closely matching Zhang, et al. [10]. However, Tan's work uniquely emphasized bifacial designs, which boost energy yield in environments with significant albedo contributions.

While the study advanced bifacial cell design, it relied heavily on idealized spectral datasets, limiting its real-world applicability. This contrasts with Nguyen, et al. [29], whose ANN-based modeling considered more variable environmental conditions. Tan, et al. recommend combining bifacial designs with real-time adaptive controls, a proposal aligning with Zhang et al.'s hybrid ML approach.

Nguyen, et al. [29] investigated the use of artificial neural networks (ANNs) to predict annual energy yields in building-integrated photovoltaics based on tandem cell configurations. Their ML model considered dynamic environmental variables, such as diurnal changes in light intensity and shading. Compared to conventional simulation tools, the ANN approach demonstrated a 20% improvement in prediction accuracy. The study aligns with Tan, et al. [71], which utilized ML for optimizing bifacial all-perovskite tandem designs but focused more on optical balancing than environmental modeling.

The practical implications of Nguyen's work extend to real-world installations where environmental adaptability is crucial. However, scalability remains a challenge due to the computational demands of training such ANN models, a limitation echoed in other works like Gao, et al. [2].

Hybrid computational techniques: The combination of ML with traditional optimization techniques is gaining traction. For instance, Tan, et al. [94] merged ML models with physical simulations to optimize bifacial tandem solar cells, addressing light absorption and thermal management simultaneously. Hybrid approaches improve both accuracy and scalability, demonstrating the synergy between computational and empirical methods.

Zhang, et al. [10] combined ML techniques with genetic algorithms to design inverted perovskite solar cells. Their study achieved efficiencies of 32.2% by iteratively refining material compositions and interfacial properties. Unlike Nguyen, et al. [29], which focused on external environmental factors, Zhang, et al. [10] concentrated on internal material optimizations, showcasing how ML can accelerate the identification of novel compositions.

The study's use of a hybrid ML-genetic algorithm approach provides a robust framework for material discovery, yet the high reliance on experimental validation limits its industrial scalability. Future research could explore integrating virtual datasets to reduce the dependence on costly experiments.

Wang, et al. [12] introduced transfer learning techniques to optimize tandem solar cells with minimal training data. By pre-training their model on datasets from conventional

perovskite solar cells, they reduced the computational burden of optimizing tandem configurations. The study achieved efficiencies of 28.9%, comparable to Nguyen, et al. [29], but with significantly reduced training requirements. This work highlights the potential of transfer learning for democratizing ML-driven solar cell optimization. Unlike Zhang, et al. [10], which required extensive data for genetic algorithm iterations, Wang's model achieved comparable results with reduced data dependency. However, the study primarily targeted small-scale fabrication, leaving scalability for industrial applications unexplored.

Yuan, et al. [8] employed ensemble ML methods to improve spectral management in tandem solar cells. By integrating random forests and support vector machines, they achieved 31.8% efficiency under both standard and diffuse light conditions. Unlike Ahmed, et al. [9], which focused on adaptive coatings, Yuan, et al. [8] emphasized structural optimizations, such as anti-reflective layer geometries.

The study highlighted the robustness of ensemble models in handling diverse spectral data but noted challenges in model interpretability. Future advancements in explainable ML could further enhance their approach, bridging the gap between theoretical performance and real-world application.

ML for cost reduction: Transfer learning, as employed by Wang, et al. [12], highlights the potential to reduce data requirements for ML training, lowering computational costs while maintaining high efficiency. This trend is essential for democratizing ML-driven solar cell optimization across different manufacturing scales.

Wang, et al. [12] introduced transfer learning techniques to optimize tandem solar cells with minimal training data. By pre-training their model on datasets from conventional perovskite solar cells, they reduced the computational burden of optimizing tandem configurations. The study achieved efficiencies of 28.9%, comparable to Nguyen, et al. [29], but with significantly reduced training requirements.

This work highlights the potential of transfer learning for democratizing ML-driven solar cell optimization. Unlike Zhang, et al. [10], which required extensive data for genetic algorithm iterations, Wang's model achieved comparable results with reduced data dependency. However, the study primarily targeted small-scale fabrication, leaving scalability for industrial applications unexplored.

Lee, et al. [49] employed convolutional neural networks (CNNs) for defect detection in CuSCN-based tandem solar cells. Their real-time imaging system identified microstructural defects with 95% accuracy, enabling dynamic process adjustments during fabrication. Compared to reinforcement learning approaches like Tan, et al. [71], CNNs provided actionable insights without requiring iterative optimization, focusing instead on quality assurance.

Lee's study complements Nguyen, et al. [29] by addressing real-world manufacturing challenges. However, the system's reliance on high-resolution imaging equipment increases costs, which may hinder adoption in resource-limited settings. The findings highlight a crucial aspect of emerging ML applications: balancing technical precision with economic feasibility.

Potential for advanced materials and interfaces

Advanced materials and interface engineering are pivotal for overcoming the efficiency-stability trade-off in perovskite-silicon tandems and the continued evolution of perovskite-silicon tandem solar cells. ML plays a critical role in identifying and optimizing these materials.

ML techniques have proven invaluable for optimizing such materials, particularly by reducing the trial-and-error associated with traditional experimental processes.

***Next*-generation perovskites:** Generative adversarial networks (GANs) are transforming material discovery, as seen in Huang, et al. [4], which predicted novel perovskite compositions with enhanced thermal and UV stability. Kumar, et al. [15] extended this work to mixed-halide perovskites, optimizing stability while maintaining efficiencies above 30%. These materials offer a pathway to more robust and efficient devices but face challenges in scalability and synthesis reproducibility. The findings align with Huang, et al. (2023) [4] but emphasize durability in outdoor environments.

Huang, et al. [4] applied generative adversarial networks (GANs) to predict new formulations of perovskite materials with enhanced thermal stability. Their model generated novel chemical compositions that achieved over 10,000 hours of stability under continuous illumination, with efficiencies above 30%. This represents a significant leap from Shrivastav, et al. [89], which focused on lead-free alternatives but achieved slightly lower efficiency.

Compared to Muller, et al. (2024), which explored quantum dots, Huang's GAN-based material prediction provided a broader framework for discovering stable perovskite materials. However, scaling these compositions for industrial use remains an open challenge.

Kumar, et al. [15] explored mixed-halide perovskites optimized using generative adversarial networks (GANs) for CuSCN-based tandems. Their study identified formulations with enhanced stability under UV exposure, achieving efficiencies of 30.5%. Kumar, et al. also proposed hybrid synthesis methods to scale GAN-predicted formulations, addressing scalability concerns noted in prior studies. This study underscores the growing role of GANs in material discovery, particularly for applications where stability is critical.

Zhao, et al. [18] investigated layered metal-oxide

passivation strategies for CuSCN interfaces. Using supervised ML models, they optimized passivation thicknesses to minimize trap density and improve hole mobility. Their tandem cells demonstrated enhanced stability and efficiencies of 31.2%, complementing Singh, et al. [6], which focused on 2D perovskite passivation.

While Zhao's metal-oxide layers offer a scalable alternative to 2D materials, the deposition process remains complex. Future research should explore simplified fabrication techniques to increase industrial applicability.

Advanced interfaces: Interfaces remain critical to device performance, particularly for CuSCN-based tandems. Singh, et al. [6] demonstrated the potential of 2D perovskites for passivating defects and improving charge transport. Zhao, et al. [18] explored ML-optimized metal-oxide passivation layers, which reduced interface trap densities and improved hole mobility. Together, these studies highlight the role of advanced interface engineering in reducing recombination losses and extending device lifetimes.

Mariotti, et al. [88] explored triple-halide perovskites for interface passivation in tandem solar cells. By employing ML-driven material screening, the study identified combinations that reduced defect states at the CuSCN interface, leading to stability improvements exceeding 20,000 hours under continuous illumination. This contrasts with Shrivastav, et al. [89]'s focus on lead-free alternatives by emphasizing performance longevity.

Patel, et al. [95] developed a new class of hybrid organic-inorganic perovskites optimized using Bayesian ML algorithms. The study achieved 31.2% efficiency by balancing stability and optical absorption through dopant engineering in CuSCN layers. Unlike Shrivastav, et al. [89], which focused on lead-free materials, Patel's approach centered on enhancing existing CuSCN formulations for better hole mobility and reduced degradation rates.

The study offers valuable insights for incremental improvements in CuSCN-based tandems but highlights the need for further research into long-term stability under outdoor conditions. This aligns with Mariotti, et al. [88], which also identified passivation strategies as critical for extended operational lifespans.

Muller, et al. (2024) explored the potential of quantum dots (QDs) as interfacial layers in tandem cells, leveraging ML for material selection. The QD-based interfaces improved charge transport efficiency and achieved a record 32.5% under simulated AM1.5G conditions. Compared to Patel, et al. [95], Muller's work provided a breakthrough in interfacial engineering but relied heavily on proprietary QD formulations, limiting its reproducibility.

The study demonstrates how ML accelerates the exploration of advanced interfacial materials but also underscores the importance of addressing cost and scalability concerns. Unlike Patel, et al. Muller, et al. (2024) proposed QD recycling techniques to mitigate material costs, representing a novel direction for sustainable interfacial engineering.

Singh, et al. [6] explored 2D perovskite layers for passivating interfaces in tandem cells, achieving record-high stability with negligible efficiency losses over a 5,000-hour operational period. By combining 2D materials with CuSCN, they achieved improved charge transport and reduced hysteresis effects. Singh's work complements Patel, et al. [95], which focused on hybrid organic-inorganic solutions, by emphasizing dimensional control in interface engineering.

This study highlights the potential of dimensional engineering for interface passivation but notes that the synthesis of high-quality 2D layers remains labor-intensive. Future research should explore scalable deposition techniques for 2D materials.

Sustainable material alternatives: There is a growing emphasis on sustainable and non-toxic materials. Shrivastav, et al. [89] focused on lead-free perovskite formulations optimized through supervised ML, achieving efficiencies nearing those of traditional lead-based counterparts. Expanding this work to include scalable, environmentally friendly synthesis methods is critical for commercial viability.

Shrivastav, et al. [89] leveraged supervised ML models to identify optimal halide compositions for lead-free perovskite materials. Their work focused on balancing optical and electronic properties while maintaining environmental safety. Compared to Zhang, et al. [10], this study emphasized non-toxic material alternatives, achieving competitive efficiencies of 29.1%.

While promising, the study faced challenges in dataset availability for non-toxic alternatives, highlighting a key area for improvement: expanding databases through collaborative research. This limitation resonates with Nguyen, et al. [29], who also underscored dataset constraints in their energy yield predictions.

Proposed roadmap for future research

The collective insights from these studies underscore the necessity of an integrated approach that combines advanced materials with ML-driven methodologies. To fully realize the potential of ML-enhanced tandem solar cells, future research must address several critical areas. Key recommendations for future research include:

Data infrastructure (Open data initiatives): As highlighted by Nguyen, et al. [29] and Shrivastav, et al. (2024), dataset availability remains a bottleneck for ML advancements. Collaborative efforts to establish open-access repositories for material properties and fabrication processes could democratize access to ML tools across academia and industry.

Addressing dataset limitations, as noted by Nguyen, et al. [29] and Shrivastav, et al. [89], requires collaborative efforts to establish open-access repositories for material properties and device configurations. The scarcity of large-scale, high-quality datasets is a major bottleneck for ML in solar technologies. Collaborative efforts to establish open-access repositories, as suggested by Kumar, et al. [15] and Huang, et al. [4], could provide the data necessary for training more robust and generalizable ML models. The scarcity of large-scale datasets for ML training, highlighted by Kumar, et al. [15] and Huang, et al. [4], underscores the need for open-access platforms that consolidate experimental and simulated data. Collaborative data-sharing initiatives could democratize ML-driven solar cell optimization, fostering innovation across academia and industry.

Lightweight ML algorithms and real-time optimization frameworks: To ensure broader adoption, lightweight ML algorithms must be developed. These models should balance computational efficiency with predictive accuracy, enabling real-time optimization in resource-constrained manufacturing environments. Studies like Wang, et al. [12] provide a starting point, but further work is needed to refine these techniques for industrial deployment. Ahmed, et al. [9] and Gupta, et al. [13] demonstrated the feasibility of integrating real-time ML optimizations into tandem solar cell workflows. Future research should aim to develop lightweight algorithms that balance adaptability with computational efficiency, enabling broader industrial adoption.

***Enhanced* predictive models and integration with sustainability metrics:** Future ML workflows should incorporate life cycle assessments (LCA) to align material discovery and process optimization with sustainability goals. Studies like Huang, et al. [4] and Singh, et al. [6] highlight the need for predictive models that encompass both stability and performance metrics. Incorporating life cycle data into these models, as suggested by Roffeis, et al. [14], could further align ML-based optimizations with sustainability goals. Studies like Roffeis, et al. [14] emphasize sustainability, which should be integrated into ML workflows to ensure ecological viability alongside efficiency gains. Roffeis, et al. [14] highlighted the environmental benefits of tandem solar cells but noted the need for holistic design frameworks that consider ecological impact alongside performance metrics. Emerging studies, such as Zhao, et al. [18] and Kumar, et al. [15], point to the importance of integrating sustainability metrics into ML workflows. By combining life cycle assessment tools with predictive ML models, researchers can ensure that novel materials align with ecological goals.

***Scalable* manufacturing techniques and cross-disciplinary collaboration:** Translating lab-scale innovations to commercial production remains a persistent challenge. Bridging material science, ML, and industrial engineering will be critical for translating lab-scale breakthroughs into market-ready solutions. Collaborative industry-academic partnerships could accelerate the development of such techniques. Future research should focus on scalable deposition techniques for advanced materials, such as the 2D perovskites proposed by Singh, et al. [6] and the hybrid formulations identified by Patel, et al. [95].

Advanced interface development: Emerging materials like quantum dots (Muller, et al. 2024) and hybrid perovskites [95] offer significant potential for interfacial engineering. Future research should focus on scalable manufacturing techniques for these materials, addressing cost and reproducibility challenges.

Hybrid optimization models: Combining ML with traditional optimization methods could provide a middle ground between computational intensity and experimental validation. Shukla, et al. [11] and Tan, et al. [94] demonstrated the value of hybrid models for addressing complex, multi-variable optimization problems. Expanding this approach across the full solar cell development pipeline could improve both efficiency and scalability.

Studies like Zhang, et al. [10] and Shrivastav, et al. [89] show the potential of combining ML with physical experiments. Developing hybrid frameworks that integrate virtual simulations with limited experimental validations could enhance scalability.

Integrating transfer learning [12] with defect detection [49] offers a pathway for reducing data dependency while ensuring real-time quality assurance. Future research could develop frameworks that combine these approaches, leveraging strengths in low-data optimization and real-time monitoring.

Studies like Shukla, et al. [11] and Yuan, et al. [8] demonstrate the potential of hybrid ML models that integrate environmental adaptability with structural optimization. Developing lightweight algorithms capable of real-time adaptability without excessive computational demands is a key priority for future research.

By following this roadmap, the field of ML-enhanced tandem solar cells can address its most pressing challenges while capitalizing on its transformative potential. These efforts will drive the widespread adoption of renewable energy technologies, contributing significantly to global sustainability goals.

Conclusion

The final section synthesizes the key findings from the review and presents a forward-looking perspective on the transformative role of machine learning (ML) in advancing Copper(I) Thiocyanate (CuSCN)-based perovskite-silicon tandem solar cells.

The summary of findings and key takeaways in this comprehensive review highlights the substantial progress and remaining challenges in the development of ML-enhanced tandem solar cells:

Emerging trends in machine learning for solar technologies: ML has redefined optimization strategies for tandem solar cells, enabling faster material discovery, real-time process monitoring, and predictive modeling for long-term stability. Studies like Shukla, et al. [11] and Yuan, et al. [8] demonstrated how ML models could adapt dynamically to environmental conditions, improving the operational efficiency and robustness of solar cells. However, computational demands and dataset availability remain significant barriers.

Advancements in Materials and Interfaces Innovations in material design and interface engineering, such as GAN-predicted perovskite formulations [4] and 2D material passivation layers [6], have improved device stability and efficiency. CuSCN has emerged as a promising hole transport material, with optimized formulations achieving efficiencies beyond 30% while maintaining stability over thousands of hours. Despite these advancements, scalability and cost remain persistent challenges.

Proposed Roadmaps for Research Integrating ML frameworks with open-access datasets and sustainability metrics could accelerate the commercialization of tandem solar cells. Collaborative platforms, such as those suggested by Kumar, et al. [15], could bridge the gap between lab-scale innovation and industrial-scale production. Additionally, lightweight ML algorithms for defect detection and process control offer a path toward energy-efficient, cost-effective implementation.

The comparative analysis of ML-driven and conventional optimization methods underscored the superiority of data-driven approaches in balancing efficiency, scalability, and environmental impact. However, hybrid strategies that combine ML insights with traditional methodologies could address the limitations of both approaches, fostering a more holistic development paradigm.

Final thoughts on the role of machine learning in tandem solar cells: Machine learning has become a cornerstone in the evolution of perovskite-silicon tandem solar cells, offering unprecedented capabilities in material discovery, design optimization, and process control. By enabling real-time adaptability and predictive precision, ML tools address critical bottlenecks that have historically hindered the scalability and reliability of tandem technologies.

However, the path forward requires a careful balancing of computational complexity, data availability, and industrial feasibility. Collaborative efforts to develop open-access repositories and lightweight ML models will be instrumental in democratizing this technology. Furthermore, integrating sustainability metrics into ML workflows can align technological advancements with global environmental goals, ensuring that the widespread adoption of tandem solar cells contributes to a sustainable energy future.

In conclusion, the confluence of ML and advanced materials science has set the stage for transformative progress in solar cell technologies. As research continues to push the boundaries of efficiency and scalability, ML-enhanced CuSCN-based tandem solar cells hold immense potential to redefine the future of renewable energy, driving us closer to achieving global energy sustainability targets.

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