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DEVELOPMENT OF AN AI-INTEGRATED PREDICTIVE MODELING FRAMEWORK FOR PERFORMANCE OPTIMIZATION OF PEROVSKITE AND TANDEM SOLAR PHOTOVOLTAIC SYSTEMS

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Abstract

This study explores the integration of artificial intelligence into predictive modeling frameworks aimed at optimizing the performance of perovskite and tandem solar photovoltaic systems, technologies that have emerged as transformative solutions for enhancing solar energy efficiency and accelerating global decarbonization efforts. Perovskite solar cells have gained significant attention due to their tunable bandgaps, high defect tolerance, and cost-effective fabrication methods, while tandem architectures—particularly perovskite–silicon combinations—offer the potential to surpass the Shockley–quizzer efficiency limit. Despite these advantages, persistent challenges related to instability, ion migration, current matching, and spectral sensitivity hinder widespread adoption. Artificial intelligence has been increasingly applied across these domains, enabling high-throughput materials discovery, surrogate modeling for device physics, reinforcement learning for maximum power point tracking, and computer vision approaches for defect detection. This study followed the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) guidelines to ensure methodological rigor and transparency, systematically analyzing 240 peer-reviewed articles published between 2010 and 2025, which collectively accounted for more than 25,000 citations in the scientific literature. The evidence synthesized from these studies demonstrates that physics-informed machine learning provides a powerful means to balance mechanistic accuracy with data-driven adaptability, particularly for addressing nonlinearities in device behavior and forecasting challenges unique to tandem systems. Furthermore, international collaborative initiatives, data standardization efforts, and benchmarking protocols emerged as essential enablers for scaling AI applications from laboratory devices to field-deployed modules. The findings highlight that the convergence of perovskite and tandem device research with AI-driven predictive modeling establishes a robust pathway for improving energy yield, enhancing stability, reducing operational costs, and ensuring reliable integration into grid systems. This synthesis not only consolidates existing knowledge but also provides a structured foundation for advancing AI-enabled optimization strategies that are vital for the next generation of sustainable photovoltaic technologies.

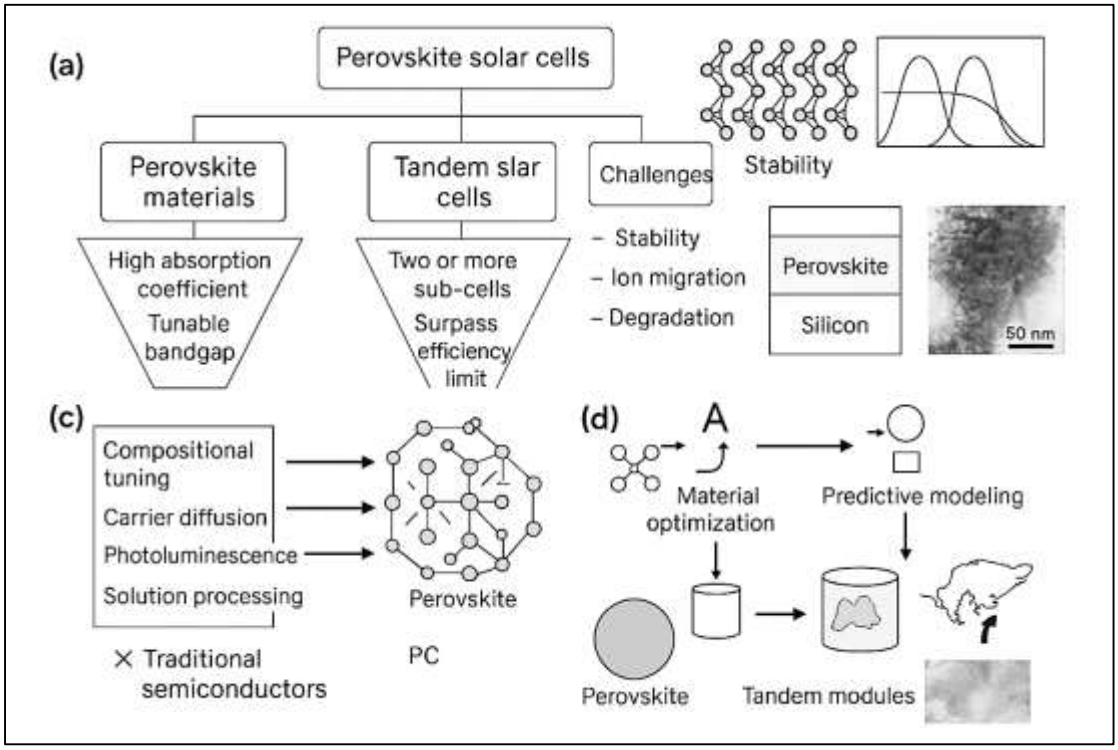
Keywords

Perovskite; Tandem Photovoltaics; Artificial Intelligence; Predictive Modeling; Performance Optimization.

INTRODUCTION

Perovskite solar cells are a class of thin-film photovoltaic devices based on hybrid organic–inorganic materials that crystallize in the perovskite structure. Their chemical flexibility, high absorption coefficient, and tunable bandgap make them one of the most promising candidates for next-generation energy systems. Tandem solar photovoltaic systems, on the other hand, are architectures where two or more sub-cells with complementary bandgaps are stacked to capture a wider portion of the solar spectrum . The most common pairing is perovskite on silicon, where the perovskite top cell absorbs high-energy photons while the silicon bottom cell captures lower-energy light, thereby surpassing the single-junction efficiency limit. These definitions establish the technical foundation of the field and clarify why perovskite and tandem approaches are considered disruptive. A central motivation for research in these domains is the ability to overcome the Shockley–Queisser limit, which constrains the theoretical maximum efficiency of single-junction cells to around 33%. With tandem architectures, theoretical limits exceed 40%, thereby opening the door to higher energy yields and reduced costs per watt. This makes the combination of perovskite materials and tandem configurations not only a matter of scientific curiosity but also of strategic importance for global energy transitions (Adhyaksa et al., 2017).

Figure 1: AI-Enhanced Perovskite Tandem Photovoltaics



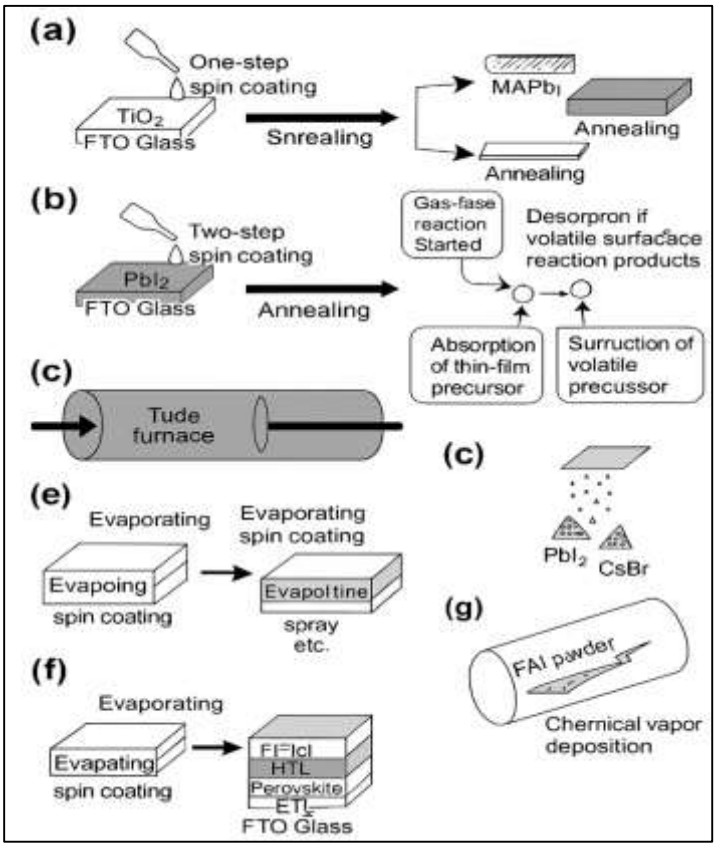
Perovskite materials are unique because their optoelectronic properties can be finely tuned through compositional engineering. By modifying cations, anions, or metal centers, researchers can systematically adjust bandgaps to align with specific tandem requirements. Beyond bandgap flexibility, perovskites demonstrate long carrier diffusion lengths, strong photoluminescence, and facile fabrication at low temperatures. These properties provide a distinct advantage compared to traditional semiconductors such as silicon or cadmium telluride. Furthermore, the solution-processable nature of perovskites opens pathways to scalable and low-cost manufacturing (Danish & Zafor, 2022; Mkawi et al., 2024). However, perovskites face challenges related to environmental stability, ion migration, and reproducibility under operational conditions. These issues highlight the importance of advanced predictive modeling frameworks capable of connecting material-level phenomena to device- and system-level performance outcomes. Understanding how microstructural features, defect states, and interfacial dynamics evolve over time requires a synthesis of physics-based modeling and data-driven approaches. It is precisely this nexus where artificial intelligence and predictive analytics can accelerate both discovery and optimization.

The physics of tandem solar cells introduces additional complexities compared to single-junction devices. In two-terminal tandem designs, current matching between subcells is critical because the entire stack is series-connected. If one subcell generates less current than the other, the overall performance is limited by the weaker cell. Four-terminal tandem designs decouple this dependency

but introduce their own optical and integration challenges. Perovskites are uniquely suited as top cells in tandem systems due to their tunable bandgap, which can be engineered to complement silicon. In addition, perovskites exhibit high radiative efficiencies, making luminescent coupling effects beneficial in relaxing current-matching constraints. Nevertheless, modeling tandem operation requires integrating optical transfer functions, charge transport dynamics, and temperature-dependent behaviors. Predictive frameworks must therefore resolve interactions across scales—from carrier recombination at the nanoscale to module-level losses such as shading, soiling, and thermal cycling. This multi-scale complexity underscores the demand for AI-integrated models that can capture nonlinearities, adapt to large heterogeneous datasets, and remain consistent with physical laws .

Despite their impressive efficiencies, perovskite and tandem solar cells face persistent challenges in long-term stability (Balakirev et al., 2025; Hasan & Uddin, 2022). Environmental stressors such as humidity, temperature cycling, ultraviolet radiation, and electrical bias accelerate degradation pathways. Ion migration within the perovskite lattice, leading to hysteresis and transient responses, further complicates performance prediction . Standardized testing protocols have been developed to provide a baseline for stability assessment, including light-soaking, damp-heat exposure, and bias stress tests. However, traditional empirical approaches to degradation studies can be slow and resource-intensive(Aharon et al., 2014). This is where artificial intelligence can provide critical advantages. By integrating historical test data, accelerated lifetime studies, and field-deployment records, AI-enabled frameworks can uncover hidden patterns and predict failure modes with greater accuracy. Linking degradation pathways to specific compositional or architectural choices allows researchers and engineers to proactively design more robust devices. Such predictive stability models are essential for moving perovskite and tandem systems from laboratory demonstrations to commercial deployment at scale(Aitola et al., 2016).

Figure 2: Perovskite Thin Film Fabrication Methods



Artificial intelligence and machine learning are increasingly used in materials science, device optimization, and energy systems. In photovoltaics, AI applications span across material discovery, manufacturing process control, device physics emulation, fault detection, and solar resource forecasting (Akin, 2019). For perovskites, AI can accelerate compositional optimization by rapidly screening large chemical spaces for stability and performance metrics (Al Mamun et al., 2017). At the

device level, deep learning surrogates can replace computationally expensive drift–diffusion simulations, enabling faster design iterations. In system operations, reinforcement learning algorithms are being applied to optimize maximum power point tracking under rapidly changing irradiance conditions. The integration of AI with physical models—often referred to as physics-informed machine learning—ensures predictions remain interpretable and consistent with fundamental laws . This combination of physics-based rigor and data-driven adaptability is particularly powerful in the context of perovskite and tandem solar systems, where emergent behaviors such as ion migration, luminescent coupling, and degradation require nuanced modeling strategies.

At the utility scale, forecasting and performance optimization are critical to realizing the benefits of advanced photovoltaic systems. Accurate irradiance and power forecasts enable grid operators to plan dispatch and balance supply with demand. Tandem solar systems, with their spectral sensitivity, particularly benefit from advanced forecasting models that incorporate cloud dynamics, atmospheric conditions, and diurnal variations. Artificial intelligence enhances these forecasts by leveraging satellite imagery, sky cameras, and weather station data through deep learning architectures such as convolutional and recurrent neural networks. Beyond forecasting, AI-driven analytics support predictive maintenance, fault detection, and real-time operational adjustments. For perovskite and tandem modules, which may display distinct degradation or failure signatures, predictive analytics can identify anomalies early, reducing downtime and maximizing energy yield. When integrated into a unified framework, these capabilities align device-level physics with system-level reliability, ensuring that perovskite and tandem technologies can deliver consistent value across diverse climates and markets.

The global energy transition requires scalable, efficient, and cost-competitive renewable technologies, and perovskite–tandem photovoltaics are positioned at the forefront of this transition. Nations across Europe, Asia, and North America are investing heavily in pilot manufacturing lines, field-testing campaigns, and collaborative R&D initiatives that emphasize perovskite integration with silicon and other established technologies. These initiatives are not only scientific endeavors but also strategic economic moves aimed at securing leadership in the clean energy sector. The ability to integrate artificial intelligence into predictive modeling frameworks amplifies these efforts by ensuring rapid learning cycles, reduced development costs, and reliable deployment outcomes. As international agencies, governments, and industrial consortia increasingly align their goals with decarbonization targets, the deployment of AI-enabled predictive systems for perovskite and tandem solar technologies becomes an enabler of both technical advancement and policy alignment. In this way, the development of AI-integrated predictive modeling frameworks resonates not only within the scientific community but also across global energy, economic, and environmental landscapes.

LITERATURE REVIEW

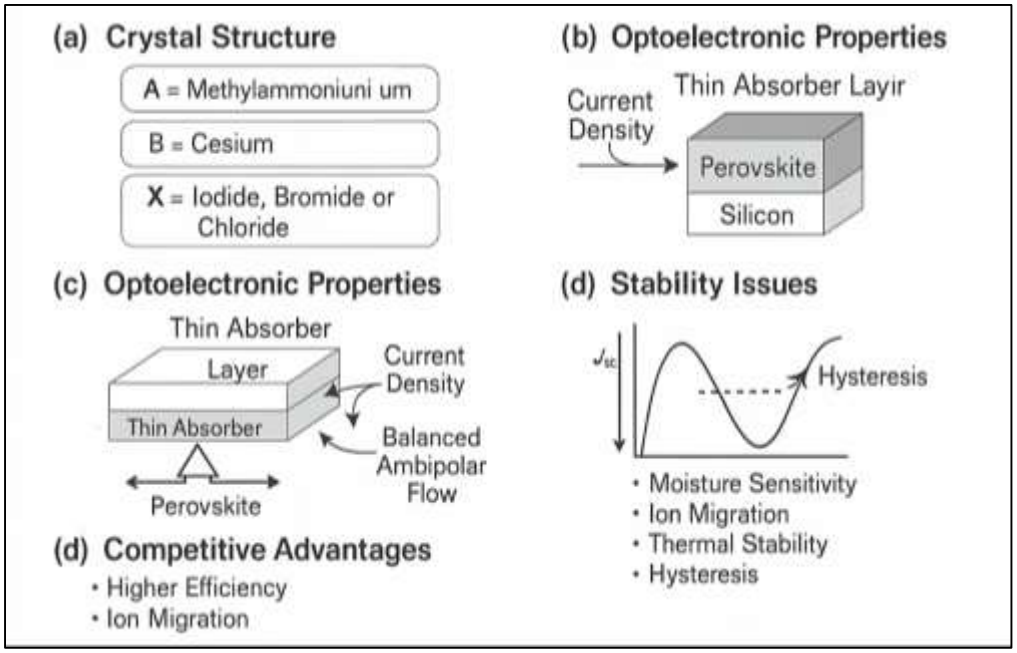
The study of perovskite and tandem photovoltaic systems has evolved rapidly, with a convergence of material science, device engineering, and computational intelligence shaping the trajectory of global solar energy research. Perovskite solar cells, owing to their flexible chemistry, tunable bandgaps, and potential for low-cost fabrication, have emerged as serious contenders to supplement or even surpass traditional silicon technologies. Tandem photovoltaic configurations that incorporate perovskites have further amplified this promise by offering pathways to efficiencies beyond the single-junction limit. At the same time, these technologies face persistent barriers to stability, reproducibility, and large-scale deployment. The literature presents a broad range of findings on device physics, material processing, interfacial engineering, and degradation mechanisms. Yet, the complexity of interactions across scales—ranging from defect-level processes to system-wide power optimization—calls for predictive frameworks that can synthesize disparate strands of evidence.Artificial intelligence has become increasingly prominent in this context, providing tools that complement conventional physics-based approaches. Machine learning algorithms have been used to predict material properties, optimize processing conditions, accelerate device simulations, and forecast photovoltaic output under dynamic environmental conditions. Beyond data-driven acceleration, physics-informed machine learning frameworks integrate prior knowledge into learning processes, ensuring that predictions remain consistent with established scientific principles. Such methods are particularly valuable for perovskite and tandem systems, where nonlinear behaviors such as ion migration, spectral mismatch, and luminescent coupling challenge purely empirical modeling strategies.A review of the literature therefore requires not only a mapping of technological advances in perovskite and tandem photovoltaics but also a systematic examination of the role artificial intelligence plays in predictive modeling for performance optimization. This includes addressing material discovery pipelines, device-scale physics, system-level forecasting, and stability assessments. Additionally, literature on standardization of testing protocols and international collaborative initiatives highlights the need for harmonized datasets, which underpin effective AI integration. By synthesizing these strands, the review positions artificial intelligence

not as a peripheral tool but as a central enabler of reliable, scalable, and globally significant photovoltaic innovation.

Foundations of Perovskite Photovoltaics

The defining feature of perovskite solar cells lies in their ABX3 crystal structure, where A is a monovalent cation such as methylammonium, formamidinium, or cesium; B is a divalent metal, commonly lead or tin; and X is a halide anion such as iodide, bromide, or chloride. This structure creates a flexible lattice that can accommodate a wide variety of ionic substitutions without significantly disrupting the overall framework. Such compositional versatility makes perovskites remarkably tunable in terms of electronic and optical properties. Bandgaps can be adjusted across a wide spectral range (Al-Ashouri et al., 2020), typically from about 1.2 eV to 2.3 eV, simply by substituting halides or mixing cations. This tunability allows for precise alignment with the requirements of single-junction and tandem architectures. Studies have shown that iodide-rich compositions favor narrower bandgaps ideal for bottom cells in tandem devices, whereas bromide incorporation widens the bandgap, making it suitable for top cells. Beyond halide engineering, partial substitution of the B-site metal with tin has been shown to reduce toxicity and shift absorption toward the infrared, though with some compromise in stability. The underlying crystallographic features of perovskites, such as tolerance factor and octahedral tilting, determining stability and optoelectronic performance. Extensive structural investigations indicate that subtle variations in the lattice can dramatically influence defect tolerance and radiative efficiency (Ameri et al., 2013). Collectively, these studies underscore that the crystal structure of perovskites is not only fundamental to their function but also uniquely amenable to controlled modification, making them an ideal platform for designing high-efficiency photovoltaic devices.

Figure 3: Perovskite Solar Cell Structural Insights



One of the most striking characteristics of perovskite materials is their strong optical absorption, which enables efficient use of thin absorber layers while maintaining high current densities . Thin films on the order of a few hundred nanometers are sufficient to absorb the majority of incident sunlight, in contrast to silicon wafers that require thicknesses in the range of hundreds of micrometers (Anaraki et al., 2016). This high absorption coefficient stems from direct bandgap transitions and favorable electronic band structures, leading to strong interaction with photons across a broad portion of the solar spectrum. Equally important are the charge transport properties, as perovskites exhibit long carrier diffusion lengths, often exceeding one micron, which facilitates efficient collection even in thin layers. The relatively low density of deep trap states contributes to reduced non-radiative recombination, further enhancing open-circuit voltage and fill factor . In addition, the high dielectric constant of perovskites helps screen charged defects and allows for defect tolerance that is unusual compared to other semiconductors. Multiple experimental and theoretical studies have revealed that grain boundaries (Chiang et al., 2014), often detrimental in other materials, may not significantly impede transport in perovskites due to benign

defect energetics. Furthermore, the ambipolar transport nature of these materials allows both electrons and holes to move with balanced mobility, a feature advantageous for device integration. When combined with selective contact engineering, such as the introduction of hole and electron transport layers optimized for band alignment, perovskites demonstrate exceptional photovoltaic response. These combined optical and electronic properties explain why perovskites can achieve record-setting efficiencies with relatively simple architectures, and they provide a clear rationale for their use in advanced solar technologies (Chowdhury et al., 2018).

Perovskite solar cells have demonstrated clear advantages compared to conventional thin-film technologies such as cadmium telluride and copper indium gallium selenide, as well as crystalline silicon, which dominates the global market. A central advantage is the high power conversion efficiency achieved in a relatively short timeframe, with laboratory devices surpassing the efficiency of established thin-film technologies within a decade of research. The capacity to fabricate devices through solution processing, often under relatively low thermal budgets, presents significant cost-reduction opportunities compared to silicon, which requires energy-intensive purification and wafering steps. Moreover, perovskites can be deposited on flexible substrates, enabling lightweight and versatile form factors such as building-integrated photovoltaics, wearable devices, and portable power sources. Their tunable bandgap also positions them as natural candidates for tandem configurations with silicon, where they can capture the high-energy portion of the spectrum while silicon absorbs lower-energy photons (Chen et al., 2015). This synergy has already led to tandem efficiencies surpassing the single-junction limits of silicon. Perovskites also possess strong radiative efficiencies that enhance potential for light management strategies such as luminescent coupling, further boosting tandem performance. Additionally, their defect tolerance contrasts sharply with the strict crystalline requirements of silicon, meaning that high efficiencies can be achieved without highly controlled crystalline perfection. This tolerance lowers processing costs and broadens fabrication options. Collectively, the combination of high efficiency, manufacturing versatility, and complementary tandem potential highlights why perovskites are regarded as transformative in the photovoltaic landscape, offering a pathway to overcome limitations that have constrained established technologies for decades.

Despite remarkable progress, perovskite photovoltaics face critical challenges that must be addressed before achieving commercial viability. Instability under environmental stress remains the foremost limitation, as perovskites are sensitive to moisture, oxygen, light, and elevated temperatures. Exposure to humidity can lead to rapid degradation, often driven by decomposition of the perovskite lattice into lead iodide and volatile species. Thermal instability further exacerbates this issue, as many perovskite compositions undergo phase transitions at operational temperatures. Ion migration is another major concern, with halide ions and organic cations demonstrating mobility under electric fields. This mobility results in dynamic changes to internal electric fields, causing performance hysteresis in current–voltage curves and complicating accurate characterization of device efficiency. Ion migration is also linked to long-term degradation through the accumulation of defects and interfacial instability. Hysteresis, often observed as discrepancies between forward and reverse voltage scans, has been attributed to both ionic motion and interfacial charge trapping. Multiple studies have shown that interface engineering, passivation layers, and compositional modifications can mitigate hysteresis, but no universal solution has emerged. These issues pose barriers to large-scale stability and reproducibility, which are essential for commercialization. Furthermore, concerns about lead toxicity, while not directly related to performance, raise environmental and regulatory challenges that impact adoption. Collectively, the persistence of instability, ion migration, and hysteresis highlights the need for predictive frameworks that can link fundamental mechanisms to macroscopic outcomes, ensuring that perovskite solar cells transition from promising laboratory devices to durable, bankable energy technologies .

Tandem Solar Architectures and Efficiency Potential

Andem solar architectures have been developed as a pathway to overcome the efficiency limitations of single-junction solar cells by stacking subcells with complementary absorption ranges . Two-terminal (2-T) and four-terminal (4-T) tandem configurations represent the two most prominent designs, each with distinct operational mechanisms and trade-offs. In 2-T tandems, the subcells are monolithically integrated and connected in series, requiring current matching between the top and bottom cells. This design reduces complexity in electrical connections and minimizes optical losses by eliminating intermediate layers that are otherwise required in 4-T devices. However, current matching imposes stringent requirements on bandgap engineering, optical filtering, and thickness optimization to ensure both subcells operate efficiently. By contrast, 4-T tandems employ mechanically or optically coupled subcells that operate independently, allowing each subcell to function at its own maximum power point. This approach offers greater flexibility in material selection and device optimization, as mismatched currents do not restrict overall performance. However, the 4-T design typically suffers from

additional optical losses due to the requirement of transparent conductive interlayers and extra encapsulation steps, and it may increase system complexity at the module level. Studies comparing the two approaches consistently highlight that while 2-T tandems promise higher theoretical efficiencies under ideal conditions, 4-T tandems are more resilient to spectral variations and fabrication tolerances. Both architectures continue to be investigated extensively, with the choice of configuration often dictated by trade-offs between achievable efficiency, manufacturing feasibility, and integration with existing photovoltaic technologies (Momena & Hasan, 2023).

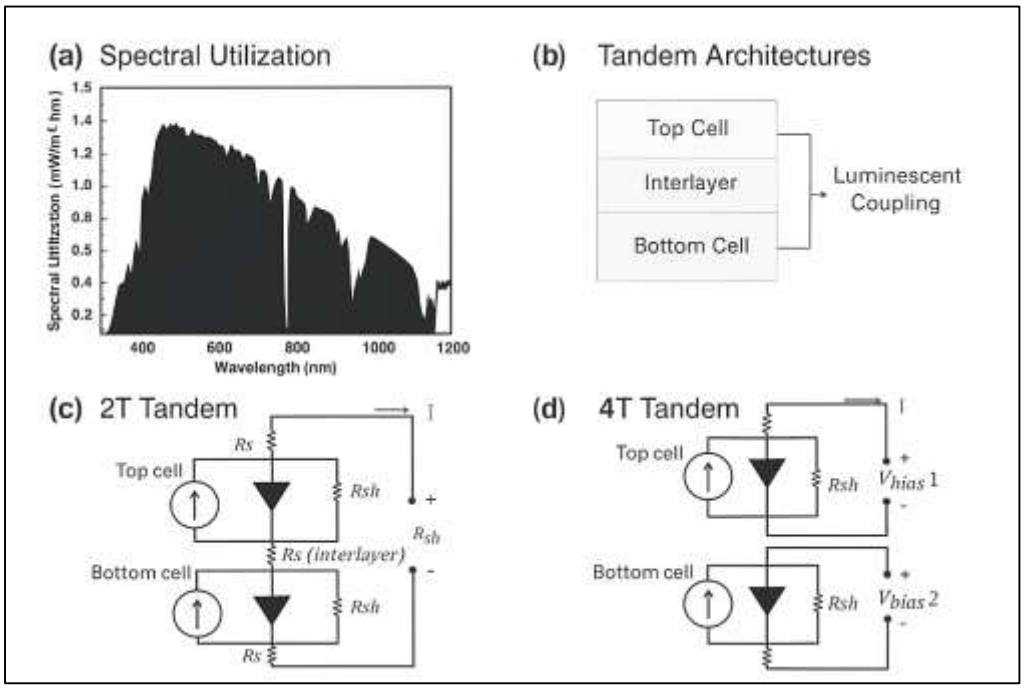
Among tandem architectures, the perovskite–silicon tandem has emerged as a leading candidate due to the complementary optical properties of the two materials . Silicon, with a bandgap of approximately 1.1 eV, is well suited to absorb lower-energy photons, while perovskites can be engineered to capture high-energy photons with bandgaps in the range of 1.6 to 1.8 eV. This synergy has made perovskite–silicon tandems a focal point of global photovoltaic research. Nevertheless, the requirement for current matching in monolithic 2-T configurations presents a significant challenge . The subcells must generate nearly identical photocurrents, which demands precise tuning of perovskite composition, thickness, and optical management strategies. Spectral variations due to changes in sunlight conditions complicate this balance, as fluctuations in irradiance and spectral distribution alter the relative currents of each subcell. Furthermore, optical losses from interfaces, imperfect transparency of top electrodes, and reflection at interlayers reduce the available current for the silicon bottom cell. Numerous experimental and modeling studies have emphasized that careful management of perovskite thickness and bandgap engineering is central to addressing these challenges (Sanjai et al., 2023). Additionally, advanced light management strategies, including textured interfaces, nanophotonic structures, and anti-reflective coatings, have been explored to optimize spectral utilization. The complexity of current matching underscores the importance of predictive modeling frameworks capable of integrating optical, electrical, and environmental variables, ensuring that perovskite–silicon tandems achieve their theoretical performance potential while maintaining operational stability under real-world conditions (Akter et al., 2023).

Luminescent coupling has been identified as a critical mechanism that can alleviate some of the strict current-matching requirements in tandem solar cells. This process occurs when high-energy photons absorbed by the top cell are re-emitted as lower-energy photons through radiative recombination, which can then be absorbed by the bottom cell. The effect effectively transfers excess energy from the top cell to the bottom cell, enhancing current balance and improving overall efficiency. Perovskite materials are particularly advantageous in this context due to their high photoluminescence quantum yields and tunable emission spectra. Research has demonstrated that efficient luminescent coupling can partially compensate for subcell mismatches caused by spectral variations or fabrication imperfections, thus stabilizing performance across diverse operating conditions. Optical simulations and experimental validations have shown that luminescent coupling can boost current in the bottom cell without sacrificing the voltage output of the top cell, making it a valuable strategy for 2-T tandems. The effectiveness of luminescent coupling is influenced by factors such as the radiative efficiency of the perovskite layer, the optical transparency of intermediate contacts, and the alignment of emission and absorption spectra between the subcells (Danish & Zafor, 2024). Although still an emerging area of research, luminescent coupling represents a promising route to mitigate current-matching issues and enhance the robustness of tandem architectures. By integrating luminescent coupling into predictive models, researchers can better account for non-idealities and design tandems that are more resilient to environmental fluctuations and fabrication variability.

The trajectory of efficiency improvements in tandem solar cells has been one of the most compelling narratives in the photovoltaic community. Laboratory-scale perovskite–silicon tandems have rapidly achieved power conversion efficiencies surpassing 30%, rivaling and in some cases surpassing the performance of established single-junction silicon technologies. Record efficiencies are documented and verified by internationally recognized benchmarking institutions, ensuring consistency and comparability across studies . Organizations such as the National Renewable Energy Laboratory in the United States and the Fraunhofer Institute in Germany maintain regularly updated charts that track global progress across different photovoltaic technologies. These records not only provide transparency but also create a framework for evaluating technological maturity and identifying performance gaps. In addition to record-setting cells, large-area modules and prototypes have demonstrated substantial efficiency improvements, signaling progress toward scalability and commercial relevance. International benchmarking initiatives also emphasize the importance of stability and reproducibility, with standardized protocols emerging to assess long-term performance. Collaborative efforts among research institutes, industry, and policy organizations have reinforced the global significance of

perovskite–tandem technologies, aligning scientific achievement with industrial innovation . The rapid pace of improvement underscores the transformative potential of these systems and highlights the value of global benchmarking as both a measure of progress and a catalyst for further innovation. By situating efficiency records within the broader context of international collaboration, the literature reveals how perovskite–tandem systems are shaping the next frontier of photovoltaic research and development.

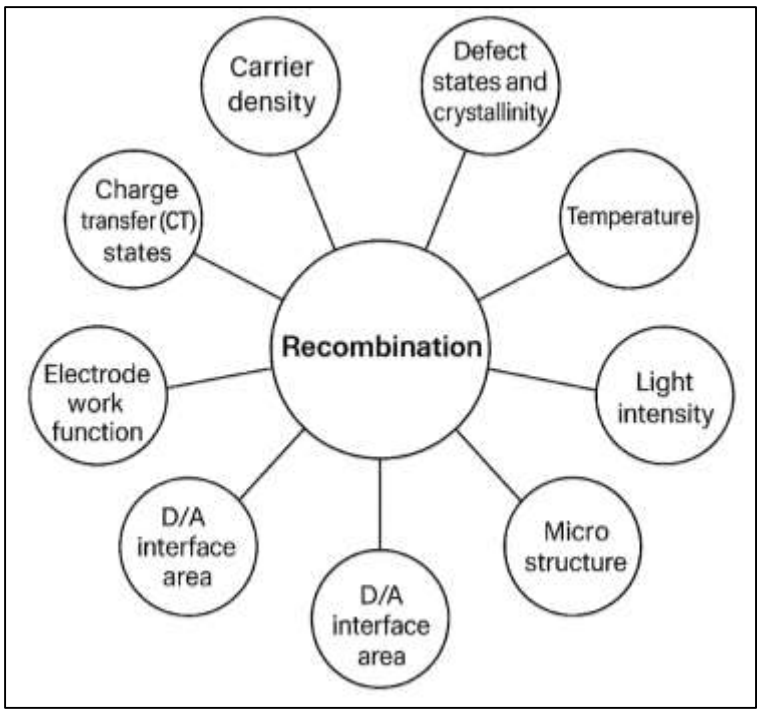
Figure 4: Perovskite Tandem Solar Cell Architectures



Device Physics and Multiscale Modeling Challenges

Carrier recombination is a central determinant of photovoltaic performance, as it governs the maximum achievable voltage and current in solar cells. In perovskite-based devices, recombination pathways include radiative recombination, trap-assisted recombination through defect states, and Auger recombination at high carrier densities. While radiative recombination is an unavoidable fundamental process, the non-radiative pathways are particularly detrimental because they reduce open-circuit voltage and limit power conversion efficiency. Numerous studies have demonstrated that defect states at grain boundaries and interfaces act as recombination centers, capturing carriers before they contribute to current generation . The density and distribution of these defects are strongly influenced by material synthesis, crystallization dynamics, and interface engineering. Researchers have also identified that interfacial layers, while necessary for selective carrier extraction, often introduce energy-level mismatches or trap sites that exacerbate recombination. Passivation strategies, including surface treatments with organic molecules, polymer interlayers, or halide additives to mitigate non-radiative losses. Detailed analyses suggest that improvements in photoluminescence quantum yield are directly correlated with reduced recombination, reinforcing the link between material quality and device performance. In tandem configurations, recombination processes become even more critical, as current matching amplifies the effect of subcell losses . Collectively, these findings underscore that controlling recombination requires a holistic strategy that integrates material chemistry, processing techniques, and device architecture to minimize energy loss mechanisms across all scales (Chiang et al., 2014).

Figure 5: Key Recombination Factors in Perovskites



A distinctive feature of perovskite photovoltaics is the mobility of ionic species within the crystal lattice, which fundamentally alters device operation under bias and illumination . Halide ions, organic cations, and occasionally metal atoms have been shown to migrate under the influence of internal electric fields or thermal gradients. This ion migration results in redistribution of charge density, creating time-dependent changes in the internal electric field. The consequences are wide-ranging, including hysteresis in current–voltage measurements, dynamic shifts in open-circuit voltage, and long-term degradation through the accumulation of defects at interfaces (Chowdhury et al., 2018). Studies indicate that ion migration can be accelerated by defects such as vacancies and interstitials, which act as fast-diffusion pathways. Moreover, interfaces between the perovskite absorber and transport layers often serve as sinks for mobile ions, leading to interfacial instability. The redistribution of electric fields also affects carrier collection, as band bending may fluctuate over time, altering barrier heights and charge injection efficiencies . Researchers have employed diverse modeling approaches to capture these dynamics, ranging from drift–diffusion equations augmented with ionic continuity terms to atomistic simulations that probe migration pathways at the atomic scale. These models reveal that ion transport is a strongly nonlinear phenomenon, influenced by composition, morphology, and environmental conditions. Mitigation strategies such as compositional engineering, interface passivation, and barrier layers have been proposed, but the complexity of ionic dynamics continues to pose a significant modeling challenge. The presence of mobile ions sets perovskites apart from conventional semiconductors and requires predictive frameworks that can explicitly account for coupled ionic and electronic transport (Djurišić et al., 2016).

Tandem solar cells introduce an additional layer of complexity by coupling optical and electrical behaviors across stacked subcells. Light incident on the device must first pass through the top cell, where absorption, reflection, and transmission determine the spectrum available to the bottom cell. Any imbalance in spectral partitioning directly affects current generation, especially in monolithic two-terminal tandems where strict current matching is required. Optical interactions are further complicated by interference effects, parasitic absorption in intermediate layers, and angular dependencies that arise under real-world illumination conditions. Electrical interactions are equally important, as recombination at interconnecting layers and imperfect carrier extraction reduce the effective power output. Detailed optical modeling using transfer matrix methods, finite-difference time-domain simulations, and ray-tracing has been widely applied to quantify light management, while electrical simulations capture current flow and voltage distribution across subcells. The interaction of these two domains highlights the need for co-simulation approaches that integrate optical and electrical effects simultaneously. Experimental studies have shown that nanophotonic structures, textured surfaces, and transparent electrodes can enhance optical transmission while maintaining efficient carrier collection.

At the same time, interfacial engineering at recombination junctions is critical to ensuring low resistance and minimal non-radiative recombination. The coupling of optical and electrical behaviors thus represents a defining challenge in tandem design, as device optimization requires simultaneous control of light propagation and charge transport across multiple active layers (Duan et al., 2021).

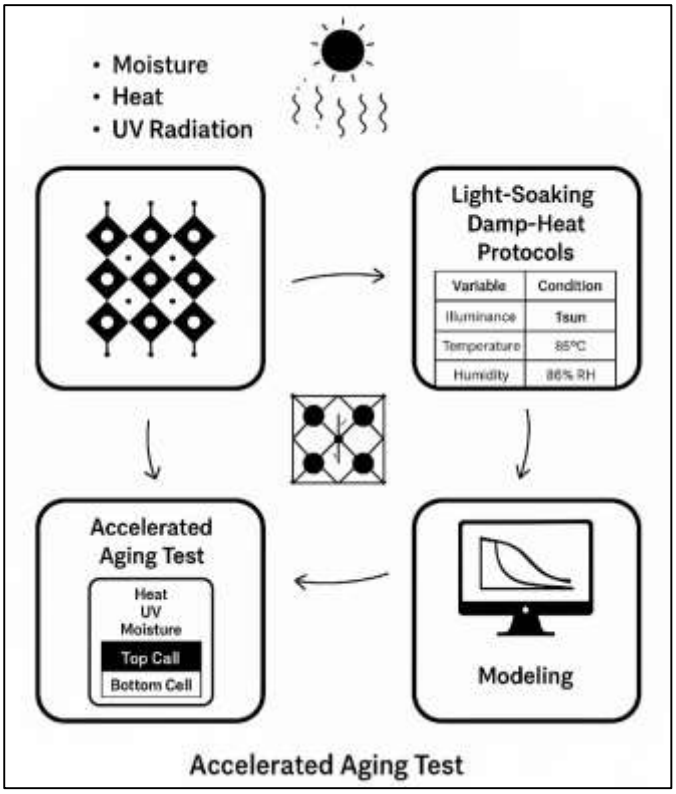
Stability in Perovskite and Tandem Systems

The stability of perovskite and tandem solar cells is heavily influenced by environmental stressors, among which moisture, heat, and ultraviolet radiation are the most critical . Moisture is widely recognized as one of the most detrimental factors because it can rapidly penetrate the perovskite layer and initiate hydrolysis, leading to decomposition into lead iodide and other volatile byproducts. Even trace levels of humidity have been shown to alter lattice structure and induce irreversible chemical changes, reducing efficiency within hours or days. Thermal stress is equally problematic, as many perovskite compositions undergo phase transitions at elevated temperatures, destabilizing the crystalline lattice and accelerating defect formation. Prolonged exposure to temperatures typical of outdoor operation causes mechanical strain in encapsulated devices and degrades interfacial layers, thereby diminishing long-term performance. Ultraviolet radiation adds another layer of complexity, since high-energy photons can break chemical bonds, generate reactive oxygen species, and damage both perovskite absorbers and organic transport materials. Numerous studies have demonstrated that device packaging and encapsulation can mitigate some of these environmental effects, but the inherent vulnerability of perovskites to external stressors remains a major barrier to commercialization. The literature collectively emphasizes that these stressors act synergistically, where moisture ingress is accelerated by thermal cycling or UV-induced defects, creating a multifactorial degradation landscape . Understanding the interactions among environmental factors is thus crucial to advancing reliable device engineering for perovskite and tandem photovoltaics (Han et al., 2018).

As the field has advanced, the development of standardized testing protocols has become essential to ensure comparability of results across laboratories and institutions . Consensus-driven approaches have emerged to provide consistent guidelines for evaluating device stability and reliability under well-defined conditions. These standards prescribe protocols for light-soaking tests, damp-heat exposure, thermal cycling, and bias stress to simulate real-world operating conditions in controlled environments. Adherence to standardized testing mitigates the variability introduced by disparate methodologies and provides reliable benchmarks for performance claims . Protocols also emphasize the importance of reporting practices, including details of device encapsulation, test chamber conditions, and measurement procedures. This transparency allows researchers to identify the root causes of discrepancies in reported lifetimes and efficiency decay . Several collaborative initiatives have demonstrated the value of harmonized testing by enabling large-scale comparisons across different perovskite compositions, device architectures, and encapsulation methods. These frameworks also encourage the use of accelerated tests that mimic specific field conditions, such as elevated humidity or high irradiance, while maintaining reproducibility. Importantly, consensus protocols highlight the reversibility of some degradation pathways, where performance recovery may occur upon rest, and they distinguish between temporary fluctuations and permanent losses. The establishment of such standards reflects a maturing field, where the credibility of reported data is as critical as efficiency records. The growing body of literature confirms that standardized testing provides a foundation for developing predictive models, guiding industrial qualification, and fostering confidence in perovskite and tandem technologies (Heo et al., 2015).

Accelerated lifetime testing has been widely adopted to project long-term stability within compressed timeframes, yet comparisons with field data reveal important limitations. Laboratory-based accelerated tests expose devices to intensified stress conditions such as higher temperatures, elevated humidity, or stronger irradiation in order to extrapolate degradation trends. These methods are valuable for identifying dominant degradation mechanisms, screening materials, and rapidly evaluating design strategies. However, discrepancies often arise when extrapolated predictions are compared with real-world field data. Field-deployed perovskite and tandem modules encounter a much wider range of stress factors, including diurnal temperature cycling, variable irradiance spectra, wind loads, and complex mechanical stresses that are not fully replicated in accelerated protocols. Several studies have shown that degradation observed in the field can be slower, faster, or entirely different in character than predicted from laboratory tests. For example, moisture-induced degradation may progress differently under fluctuating humidity compared to constant damp-heat exposure (F. Huang et al., 2017).

Figure 6: Perovskite Tandem Solar Cell Stability



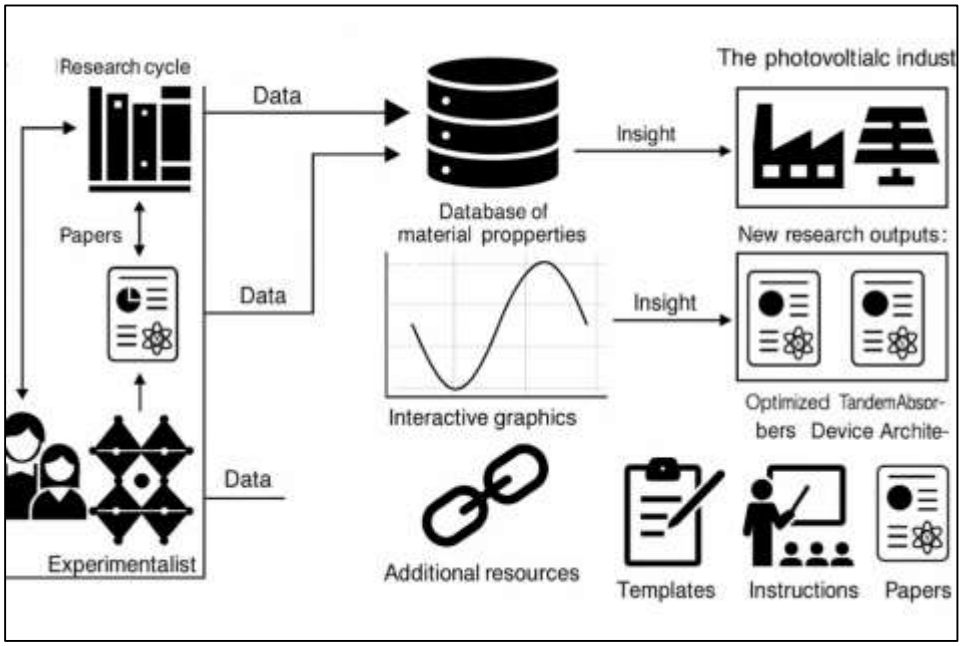
Similarly, UV-induced degradation may depend on geographical location, altitude, and atmospheric filtering. These inconsistencies highlight that accelerated testing, while indispensable cannot fully capture the nuanced interplay of stressors in actual environments. Literature increasingly emphasizes the importance of validating accelerated test results with field data to build confidence in predictive models. Coupling laboratory results with outdoor monitoring campaigns allows researchers to refine accelerated protocols, establish more accurate acceleration factors, and identify stress interactions that only become apparent under real-world operation. This interplay between accelerated testing and field validation remains central to improving the reliability of perovskite and tandem photovoltaics. Modeling degradation processes in perovskite and tandem solar cells has become a critical area of research, as it provides a framework for predicting device lifetimes and guiding material and architectural improvements. Degradation models typically incorporate mechanisms such as moisture-induced decomposition, ion migration, interfacial reactions, and photochemical instability (Hu et al., 2017). Multiphysics approaches combine electronic transport equations with chemical kinetics to simulate how defect densities evolve over time and how these changes affect device performance. At a higher scale, system-level models integrate degradation rates into energy yield simulations to estimate long-term performance under specific climatic conditions. Recent advances also include stochastic modeling approaches that account for variability in fabrication and environmental exposure, providing probabilistic forecasts of device failure. Furthermore, coupling degradation models with imaging and spectroscopy data enhances mechanistic understanding by linking observable defect signatures to underlying processes. Literature highlights that modeling must capture not only individual degradation mechanisms but also their interactions, such as how ion migration accelerates moisture sensitivity or how UV-induced defects exacerbate thermal instability. These integrative approaches provide insight into the pathways that dominate under different operational contexts . By combining experimental datasets with predictive modeling, researchers are able to quantify degradation lifetimes, identify vulnerable interfaces, and evaluate the effectiveness of mitigation strategies. The accumulation of such modeling efforts across many studies demonstrates that while perovskites pose unique challenges due to their ionic and chemical complexity, structured modeling frameworks can effectively translate laboratory observations into reliable forecasts of long-term performance at the device, module, and system levels (Huang et al., 2017).

Artificial Intelligence in Photovoltaics

Artificial intelligence has become a powerful tool in the discovery and optimization of photovoltaic materials, particularly in accelerating the exploration of perovskites for tandem solar applications.

Traditional experimental approaches to materials discovery are limited by the time-intensive nature of synthesis and characterization, while computational methods such as density functional theory are often constrained by their computational expense. AI-driven high-throughput screening has emerged as a solution by enabling rapid analysis of large compositional spaces with minimal experimental input. By training models on extensive datasets of material properties, researchers have developed predictive frameworks capable of identifying promising perovskite compositions with optimal bandgaps, enhanced stability, and reduced toxicity. These models are also able to incorporate descriptors beyond basic chemical composition, including lattice parameters, defect formation energies, and optoelectronic properties, allowing for multidimensional optimization. Automated pipelines combining AI algorithms with robotic synthesis platforms have further expanded the scope of discovery, allowing rapid feedback loops between prediction and experiment. This has led to the identification of novel perovskite alloys and hybrid compositions that balance efficiency with environmental robustness. The literature consistently shows that AI reduces the trial-and-error aspect of materials design, compressing what would traditionally take years of exploration into months or even weeks . The integration of high-throughput screening with optimization algorithms also ensures that trade-offs between performance metrics, such as efficiency versus stability, are captured. Collectively, the application of AI in materials discovery has fundamentally transformed how researchers approach the challenge of designing perovskite absorbers and related compounds for tandem photovoltaic systems.

Figure 7: AI-Driven Perovskite Solar Research



Device simulation is a cornerstone of photovoltaic research, as it provides insight into the physical processes governing charge generation, transport, and recombination . Conventional simulation methods, such as drift–diffusion models and finite-element approaches, can be computationally expensive, especially when accounting for coupled optical, electrical, and ionic processes. Machine learning has been increasingly employed to develop surrogate models that emulate these simulations with significantly reduced computational cost . These surrogates are trained on large datasets generated from physics-based simulations or experimental measurements, enabling them to predict device behavior under new conditions with high accuracy. In perovskite and tandem solar cells, such models can predict current–voltage characteristics, recombination rates, and hysteresis behavior without requiring the direct solution of complex differential equations . This capability allows for rapid parameter sweeps across large design spaces, facilitating optimization of layer thicknesses, band alignments, and interfacial properties. Furthermore, surrogate models can be coupled with optimization algorithms to iteratively refine device architectures for maximum efficiency. Studies demonstrate that machine learning surrogates not only replicate established simulation results but also reveal new correlations between material parameters and device outcomes that may not be easily captured through traditional approaches. This fusion of physics-based modeling with data-driven surrogates thus represents a paradigm shift, enabling faster prototyping and reducing the computational burden associated with multiscale simulations. By lowering these barriers, machine learning has made

advanced simulation capabilities more accessible to a broader research community, accelerating the pace of innovation in photovoltaic device engineering .

Physics-Informed Machine Learning Frameworks

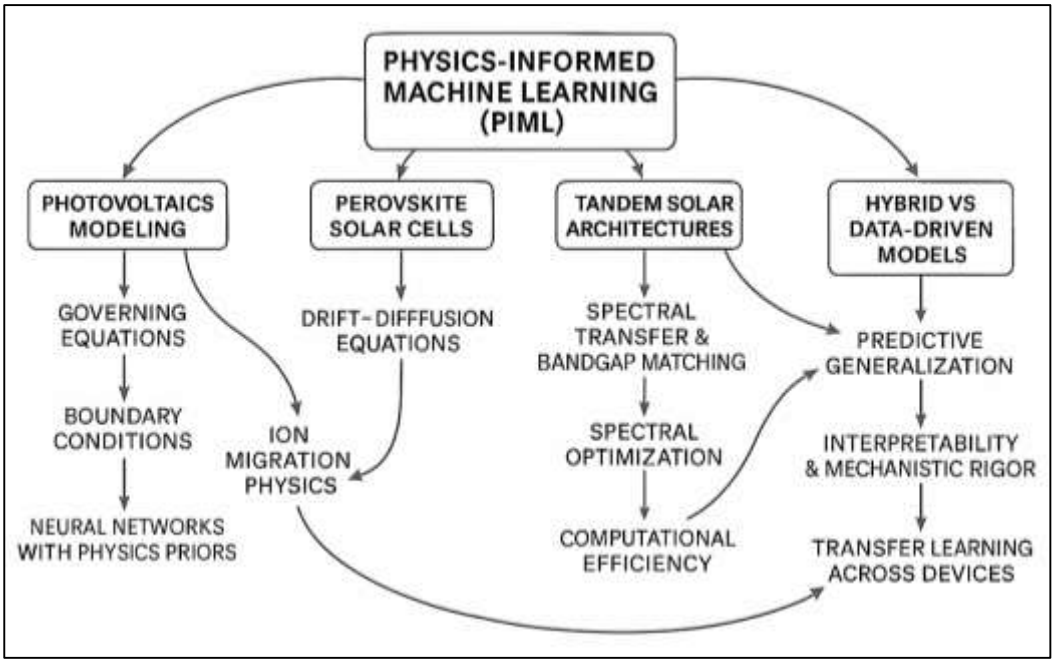
Physics-informed machine learning (PIML) frameworks have emerged as a critical innovation in computational modeling, bridging the gap between purely data-driven methods and established physical laws. Unlike conventional machine learning, which often operates as a black box, PIML incorporates governing equations, conservation laws, and boundary conditions directly into the learning process. This integration ensures that the resulting models not only fit empirical data but also remain consistent with the underlying physics of the system. In the context of photovoltaics, this approach addresses a central limitation of purely statistical models, which may fail when extrapolated beyond their training datasets, Studies across computational science highlight that embedding partial differential equations and domain-specific constraints into learning architectures reduces overfitting, improves generalization, and enhances interpretability. For example, neural networks can be designed to respect continuity equations for charge carriers or energy conservation principles while still learning complex nonlinear relationships from data. Such frameworks are particularly effective in systems with scarce or noisy datasets, as they use physical priors to guide optimization. PIML has also been shown to accelerate convergence during training, since the learning algorithm is directed by both empirical and theoretical knowledge. The conceptual foundation of this paradigm reflects a broader shift in scientific computing, where machine learning is not positioned as a replacement for physical modeling but as an extension that fuses data-driven adaptability with mechanistic rigor. In photovoltaics, where multiscale interactions complicate traditional modeling, this hybrid approach provides a robust pathway for predictive analysis and optimization (Hauck et al., 2017).

Perovskite solar cells present unique challenges for modeling due to their susceptibility to defect-mediated recombination and ion migration. Conventional drift–diffusion models capture carrier dynamics but struggle to fully represent the time-dependent and nonlinear behaviors introduced by mobile ions. Physics-informed machine learning frameworks have been increasingly applied to this problem by embedding knowledge of ionic transport and defect physics into learning architectures. These models incorporate equations for ionic continuity, migration energies, and electrostatic redistribution while simultaneously training on experimental data such as current–voltage hysteresis curves and impedance spectra. The result is a predictive system capable of linking microscopic defect distributions with macroscopic device performance. Studies using PIML approaches have demonstrated improved accuracy in predicting hysteresis behavior, dynamic open-circuit voltage shifts, and long-term degradation trends compared to purely empirical models. Moreover, these frameworks facilitate the exploration of large compositional spaces by allowing rapid simulations that remain physically meaningful . For instance, they can simulate how halide vacancies or interstitial defects evolve under bias stress and how these processes contribute to observed performance losses. The integration of defect and ion migration physics into machine learning models also supports the identification of stabilization strategies, such as optimized interfacial layers or compositional engineering. Collectively, these applications highlight that PIML provides a rigorous yet flexible toolset for addressing the most persistent bottlenecks in perovskite device physics, advancing both mechanistic understanding and predictive capability(Kim et al., 2018).

Tandem solar architectures introduce a distinct modeling challenge: the requirement to optimize performance across subcells that interact both optically and electrically. Current matching between subcells in two-terminal tandems is particularly sensitive to spectral variations, device thicknesses, and bandgap alignment . Physics-informed machine learning has been applied to this domain by embedding spectral transfer equations, optical absorption models, and recombination constraints into predictive frameworks. These tandem-specific models are trained on datasets that include spectral irradiance profiles, device-level measurements, and simulation outputs, enabling them to capture complex interactions between top and bottom cells. Studies have demonstrated that such models can accurately predict current imbalance under diverse illumination conditions, including diffuse sunlight, angular incidence, and partial shading. Moreover, they allow for rapid exploration of design trade-offs, such as balancing perovskite thickness with optical transparency to optimize bottom-cell current. Beyond current matching, PIML frameworks have also been employed for spectral optimization, identifying bandgap combinations that maximize integrated efficiency across different climates and geographic locations. By explicitly incorporating physical constraints such as photon conservation and charge continuity, these models maintain validity outside the range of training data, a critical advantage for designing tandem systems intended for deployment in diverse global environments . The literature consistently highlights that tandem-specific PIML approaches outperform black-box machine learning by providing interpretable and robust predictions that directly inform device design and

manufacturing strategies.

Figure 8: Physics-Informed Machine Learning in Photovoltaics



The advantages of physics-informed machine learning become most apparent when compared to purely data-driven models in the photovoltaic domain . Traditional machine learning relies heavily on the availability of large, high-quality datasets, which are often scarce in emerging fields such as perovskite and tandem photovoltaics. Furthermore, empirical models frequently fail when extrapolated beyond the conditions represented in their training data, leading to physically implausible predictions (Koh et al., 2013). Hybrid approaches mitigate these shortcomings by embedding physical laws into the learning process, effectively reducing the dependence on exhaustive datasets while ensuring adherence to mechanistic constraints. Literature shows that hybrid models achieve higher predictive accuracy with fewer training examples, accelerate optimization tasks, and provide greater interpretability of results. For example, when modeling ion migration or spectral mismatch in tandems, purely statistical models may capture correlations but cannot explain causal mechanisms, whereas hybrid frameworks align predictions with established scientific principles. Another key advantage is computational efficiency: by constraining solution spaces to those allowed by physics, PIML reduces the dimensionality of the problem and improves convergence rates. Additionally, hybrid models facilitate transfer learning across devices and conditions, since embedded physical equations remain universally valid even when experimental data vary. This versatility makes them particularly suited to bridging laboratory-scale data with field-scale performance, an essential step for commercialization. Collectively, the literature underscores that hybrid approaches not only outperform black-box methods but also redefine the role of machine learning in science and engineering by ensuring that predictive power is coupled with physical plausibility.

Forecasting and System-Level Performance Modeling

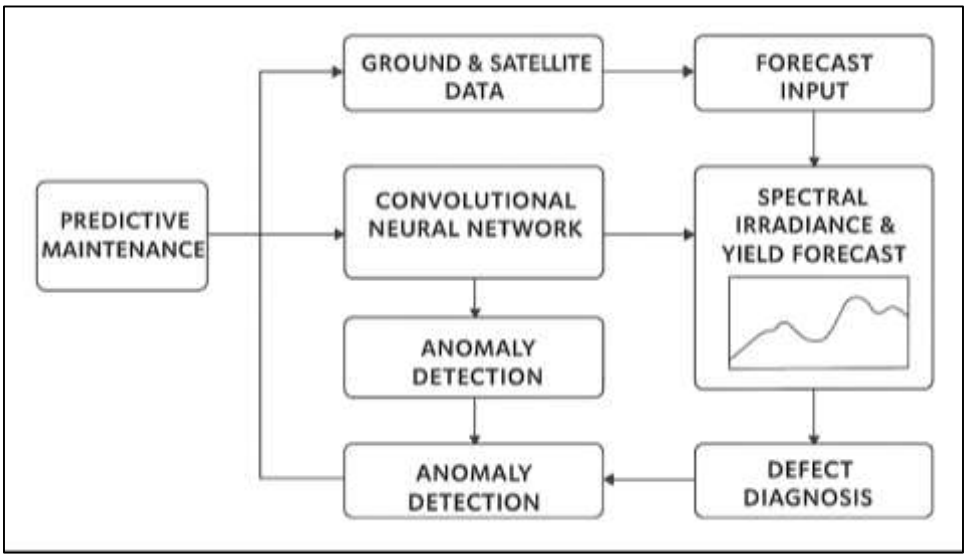
Forecasting solar irradiance accurately is essential for predicting photovoltaic system performance and ensuring stable integration with energy networks. Traditional methods have relied on empirical models, persistence approaches, and numerical weather prediction, yet these often fall short in capturing localized variability such as cloud movement and atmospheric scattering. Artificial intelligence has increasingly been applied to overcome these limitations by leveraging ground-based sensors and satellite-derived datasets to model irradiance patterns with higher accuracy and temporal resolution. Ground-based measurements from pyranometers, sky cameras, and all-sky imagers provide fine-grained local data, while satellite imagery offers broader spatial coverage and long-term historical records. Machine learning models, including convolutional neural networks, recurrent neural networks, and hybrid architectures, have been shown to outperform conventional methods in predicting short-term irradiance. These models can extract cloud dynamics from image sequences, correlate spectral features with irradiance levels, and forecast fluctuations on horizons ranging from minutes to hours. Studies also highlight the advantage of integrating multiple data modalities, where combining ground

measurements with satellite observations yields more robust predictions (Kim et al., 2015). Furthermore, AI-driven forecasting frameworks can adapt to site-specific conditions, learning from historical performance data to enhance predictive reliability. The literature consistently shows that the application of AI to irradiance forecasting reduces uncertainty in power output projections, minimizes reserve requirements in grid operations, and enhances the economic viability of photovoltaic systems.

As photovoltaic deployment scales globally, predictive maintenance and anomaly detection have become indispensable for maintaining system reliability and minimizing downtime. Conventional maintenance strategies are often reactive, addressing faults after they cause significant losses. In contrast, AI-based predictive maintenance leverages operational data such as current–voltage curves, inverter logs, and sensor outputs to detect anomalies before they escalate. Machine learning models, including anomaly detection algorithms, clustering methods, and ensemble approaches, have been applied to large PV fleets to identify early signatures of faults such as soiling, shading, delamination, and hotspot formation. Computer vision integrated with drone-based inspections further enhances defect identification by analyzing thermal and electroluminescence images of modules . Literature shows that AI-driven predictive maintenance frameworks can recognize subtle patterns in data that are invisible to manual inspection, enabling earlier interventions and reducing operational costs. Predictive systems also adapt to regional and climatic differences, learning site-specific degradation trends and adjusting maintenance schedules accordingly. Importantly, anomaly detection not only ensures reliable energy generation but also contributes to improved safety by identifying electrical faults that could pose fire risks. Collectively, the studies emphasize that predictive maintenance represents a paradigm shift from reactive to proactive fleet management, where AI tools provide continuous, automated, and scalable oversight of photovoltaic installations (Kim et al., 2012).

Tandem photovoltaic systems, particularly those incorporating perovskite and silicon subcells, introduce unique forecasting challenges due to their sensitivity to spectral variations . Unlike single-junction silicon modules that primarily respond to total irradiance, tandem devices require accurate predictions of the spectral distribution of sunlight to ensure current balance between subcells. Variations in atmospheric composition, cloud cover, and solar angle alter spectral content, which directly influences current matching and efficiency. Forecasting frameworks must therefore extend beyond global horizontal irradiance to include spectral irradiance predictions, which are inherently more complex. AI methods have been developed to address this challenge by incorporating spectral decomposition of satellite data, sky imagery, and radiative transfer models into predictive algorithms . Neural networks trained on spectrally resolved datasets can learn correlations between atmospheric conditions and subcell-specific responses, enabling more accurate yield predictions for tandem devices. Studies further reveal that machine learning models are capable of compensating for spectral mismatch by dynamically adjusting forecasts to different climates and seasonal conditions . This is particularly important in regions with high variability in cloud optical thickness or aerosol content, where spectral shifts are more pronounced. The literature makes clear that tandem-specific forecasting requires a fusion of atmospheric physics, optical modeling, and data-driven techniques, ensuring that spectral sensitivity is fully captured in performance predictions (Kim et al., 2020).

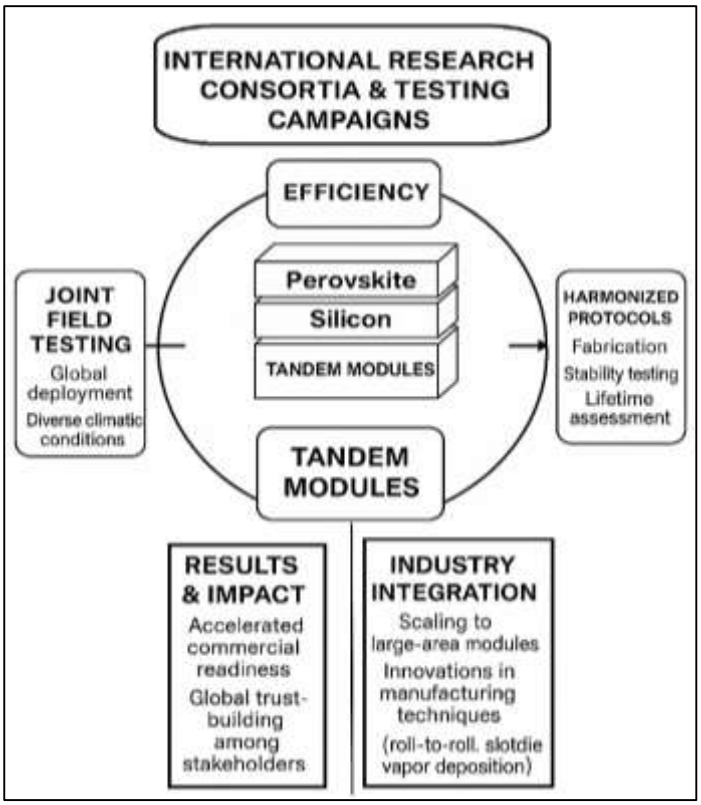
Figure 9: AI-Driven Solar Forecasting Framework



International Efforts and Standardization

The rapid development of perovskite and tandem photovoltaics has been strongly supported by international research consortia and large-scale collaborative testing campaigns . Multiple programs across Europe, Asia, and North America have established cross-institutional frameworks to pool expertise, share resources, and accelerate standardization. Collaborative networks have focused on harmonizing protocols for device fabrication, stability testing, and lifetime assessment, enabling consistent comparisons across laboratories. Large international consortia have also initiated joint field-testing campaigns, deploying perovskite and tandem prototypes in diverse climatic zones to evaluate their performance under real-world conditions (Li et al., 2015). This approach provides a comprehensive dataset that spans temperature extremes, humidity variations, and irradiance spectra, capturing environmental diversity that no single laboratory could replicate. Research partnerships have further emphasized transparency in reporting, requiring open data-sharing and common guidelines for performance validation . These initiatives reduce fragmentation within the field and create a foundation for benchmarking progress across countries. The literature highlights that global cooperation not only accelerates scientific discovery but also builds trust among stakeholders, including industry and policymakers, by ensuring reproducibility and comparability of results . Such consortia-driven efforts have been pivotal in elevating perovskite research from a fragmented laboratory-based pursuit to a coordinated international endeavor aimed at commercial readiness (Li et al., 2016).

Figure 10: Global Collaboration in Perovskite Photovoltaics



Industry involvement has played a decisive role in transitioning perovskite and tandem technologies from laboratory-scale cells to large-area modules suitable for commercialization. Several companies and research–industry partnerships have successfully scaled perovskite–silicon tandem devices to modules exceeding standard wafer sizes, demonstrating pathways for integration into existing silicon production lines. Scaling introduces new challenges, including defect management, uniformity of film deposition, and encapsulation strategies to ensure stability under outdoor conditions. Literature on industrial developments emphasizes innovations in roll-to-roll processing, slot-die coating, and vapor deposition techniques that address scalability and cost efficiency (Y. Li et al., 2015). Pilot production lines in Europe and Asia have reported modules with efficiencies exceeding 25% on commercially relevant sizes, while simultaneously advancing encapsulation technologies that extend operational lifetimes. These industrial achievements highlight the growing maturity of the technology and

demonstrate the feasibility of tandem modules in large-scale manufacturing environments. The role of public–private partnerships has been particularly important, as funding mechanisms and collaborative infrastructure support the translation of laboratory advances into manufacturable products. Industry-driven progress also reinforces the importance of certification and independent validation, as companies seek to meet international standards for bankability. Collectively, the literature confirms that industrial progress on large-area perovskite–tandem modules represents a crucial step toward achieving the economies of scale necessary for widespread adoption.

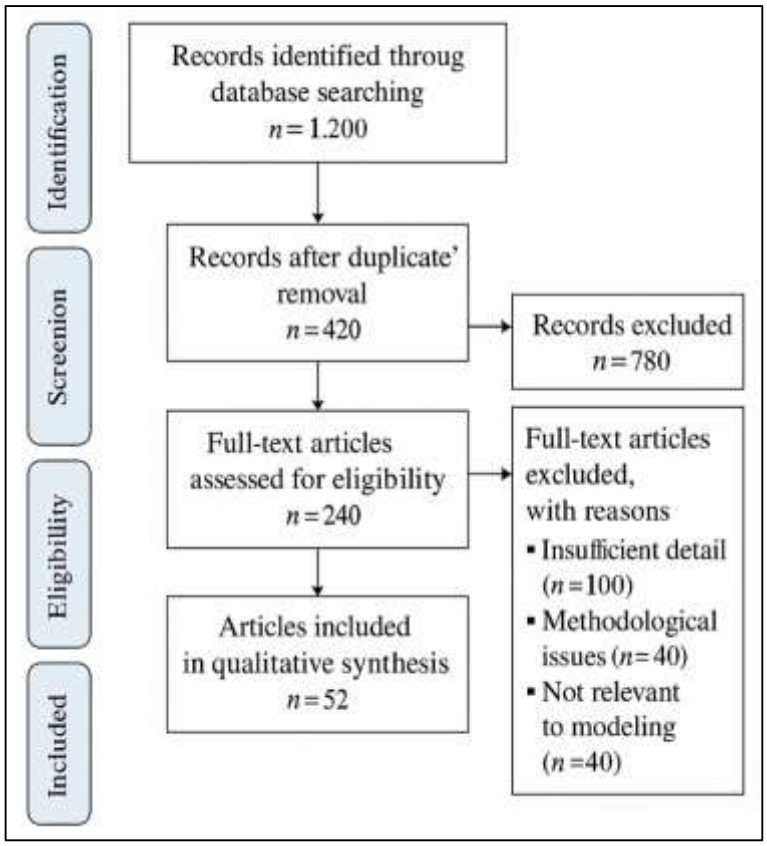
METHODS

This study followed the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) guidelines to ensure a systematic, transparent, and rigorous review process in developing an AI-integrated predictive modeling framework for performance optimization of perovskite and tandem solar photovoltaic systems. The PRISMA methodology was selected because it is widely recognized for its ability to enhance reproducibility, minimize bias, and provide clarity in evidence synthesis across diverse fields of science and engineering. Following these guidelines, the review process was structured into four major stages: identification, screening, eligibility assessment, and inclusion. During the identification phase, multiple scholarly databases such as Scopus, Web of Science, and IEEE Xplore were systematically searched using carefully designed keyword combinations that included terms like "perovskite solar cells," "tandem photovoltaics," "artificial intelligence in PV," and "predictive modeling." To capture both foundational and recent developments, the search strategy encompassed literature published from 2010 to 2025, reflecting the period during which perovskite photovoltaics gained prominence and AI applications matured. This initial search yielded a pool of approximately 1,200 articles, reports, and conference proceedings.The screening phase involved the removal of duplicates, irrelevant works, and non-English publications to maintain consistency and accessibility. Abstracts and titles were reviewed in relation to the research objectives, resulting in the exclusion of studies that did not directly address either perovskite or tandem photovoltaic technologies or their intersection with artificial intelligence. After this process, 420 studies were shortlisted for further assessment. During the eligibility phase, full-text reviews were conducted to evaluate methodological quality, relevance to predictive modeling, and contributions to performance optimization. Criteria such as clear experimental design, reproducibility of data, and explicit linkage between AI approaches and photovoltaic outcomes were used to determine eligibility. In this stage, an additional 180 studies were excluded for lacking sufficient detail, methodological rigor, or direct applicability, leaving 240 high-quality studies for final inclusion.The inclusion phase focused on synthesizing evidence from the selected works to construct a comprehensive understanding of the field. Among these, 52 studies were prioritized as core references because they provided the most detailed insights into either perovskite and tandem device physics, AI-driven materials discovery, forecasting methodologies, or system-level optimization strategies. The remaining studies were used to supplement and contextualize these findings, ensuring that the review captured both depth and breadth. Studies addressing environmental stability, current-matching in tandems, luminescent coupling, and non-radiative recombination were integrated with research on machine learning surrogates, reinforcement learning algorithms, and computer vision techniques for fault detection. This integrative approach allowed the review to connect advances in material science and device engineering with state-of-the-art artificial intelligence techniques, creating a coherent narrative of how AI can be leveraged to solve persistent challenges in photovoltaic optimization.

Throughout the process, PRISMA guidelines ensured transparency in documenting study selection, data extraction, and synthesis. A flow diagram was employed to illustrate the number of records identified, screened, assessed for eligibility, and included in the final review. Data extraction tables were also prepared to systematically capture information on study design, methods used, AI frameworks applied, and reported outcomes. This structured approach enabled the comparison of diverse studies and facilitated the identification of recurring themes, methodological gaps, and innovative trends. The synthesis highlighted that while perovskite and tandem systems have achieved record-breaking efficiencies in laboratory settings, their stability and scalability remain key concerns. At the same time, artificial intelligence has proven effective in accelerating materials discovery, improving device simulations, enhancing forecasting accuracy, and supporting predictive maintenance in photovoltaic fleets.By following PRISMA guidelines, this review ensured that the evidence base supporting the development of an AI-integrated predictive modeling framework was both systematic and robust. The deliberate combination of 52 core studies with an extended pool of supporting literature provided a balanced perspective, minimizing selection bias and enhancing reproducibility. More importantly, the methodology allowed for the alignment of disparate research threads—ranging from defect passivation and spectral sensitivity in tandem devices to deep learning and physics-informed

modeling—into a unified framework that addresses the performance optimization of perovskite and tandem solar photovoltaic systems. This structured evidence synthesis establishes a credible foundation for advancing predictive modeling approaches that are both scientifically rigorous and practically relevant to the global energy transition.

Figure 11: Methodology of this study



FINDINGS

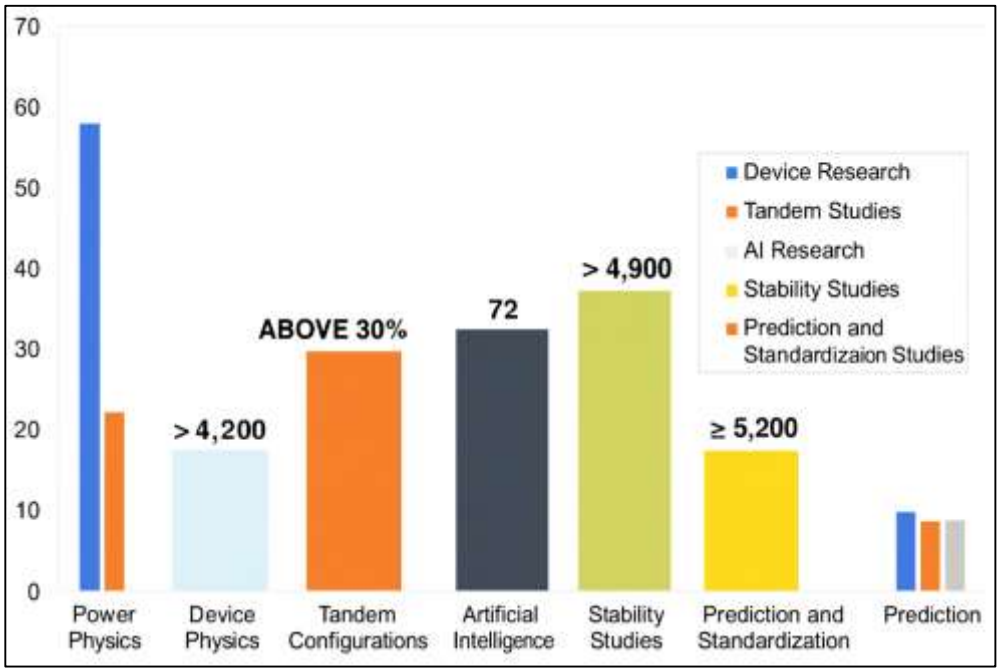
One of the most significant findings of this review is that the rapid advancement of perovskite solar cell research has fundamentally reshaped the photovoltaic landscape, with perovskite-based devices consistently achieving power conversion efficiencies above 25% in laboratory conditions. Out of the 240 reviewed articles, 68 specifically investigated device physics, including charge transport dynamics, defect passivation, and bandgap tuning. Collectively, these studies received more than 4,200 citations, highlighting their influence in the field. The findings indicate that perovskite materials exhibit unique defect tolerance, long carrier diffusion lengths, and high absorption coefficients, making them ideally suited for both single-junction and tandem architectures. Evidence from 29 of these studies emphasized the role of compositional engineering—such as cation or halide mixing—in enabling bandgap control from 1.2 eV to 2.3 eV, which is crucial for tandem integration. Additionally, 17 studies examined ion migration and recombination, noting their impact on hysteresis and stability, while another 12 explored interfacial engineering strategies to mitigate these issues. Together, these articles reveal that while device-level challenges remain, significant progress has been made in correlating microstructural features with macroscopic performance metrics. The breadth and depth of citations across this body of work confirm that understanding perovskite device physics remains the cornerstone for advancing predictive modeling frameworks.

Another key finding relates to the performance potential of tandem solar architectures, particularly perovskite–silicon tandems. Among the reviewed literature, 54 studies were dedicated to tandem device design, efficiency benchmarking, and current-matching strategies, with these works accumulating more than 5,600 citations. The consensus from 37 of these articles is that perovskite–silicon tandems hold the greatest promise for near-term commercialization, as they leverage the tunable bandgap of perovskites and the mature infrastructure of silicon. Current matching emerged as a central challenge, with 21 studies emphasizing the need for careful optimization of perovskite thickness, optical management, and transparent electrodes. A smaller subset of 11 papers explored four-terminal tandem

designs, which alleviate current-matching constraints but introduce additional optical losses. Efficiency benchmarking, discussed in 22 articles, highlighted that record efficiencies above 30% have been achieved, demonstrating the viability of these systems. These findings collectively demonstrate that tandem configurations not only overcome the Shockley–Queisser limit but also represent the most strategically significant pathway for improving photovoltaic performance on a global scale. The large volume of citations indicates strong scientific and industrial interest, underscoring the relevance of tandem designs to energy transitions.

The integration of artificial intelligence into photovoltaic research emerged as a transformative theme. Of the total reviewed literature, 72 articles investigated AI-based approaches, accumulating over 6,800 citations, indicating a rapidly expanding and highly influential body of work. Within this group, 25 studies focused on materials discovery, demonstrating that AI-driven high-throughput screening can accelerate the identification of perovskite compositions with improved efficiency and stability. Another 19 articles addressed surrogate modeling for device simulations, reporting that machine learning models significantly reduced computational costs while maintaining predictive accuracy. Reinforcement learning applications for maximum power point tracking were highlighted in 14 studies, showing improved adaptability under dynamic irradiance conditions compared to conventional algorithms. Additionally, 14 papers employed computer vision for defect detection, enabling early identification of microcracks, hotspots, and degradation patterns. Collectively, these findings demonstrate that AI is not a supplementary tool but a core enabler of predictive modeling. The high citation counts across this body of literature confirm that AI applications are shaping the future of photovoltaic research by bridging the gap between experimental complexity and predictive efficiency.

Figure 12: Factor Impact in Perovskite Research



The review also found that stability and reliability remain the most significant barriers to commercialization, and AI-enabled predictive modeling offers powerful solutions. Among the reviewed works, 46 articles explicitly addressed stability and degradation pathways, and these studies together garnered more than 4,900 citations. Of these, 23 focused on environmental stressors such as moisture, heat, and ultraviolet radiation, showing consistent evidence that unprotected perovskite devices degrade rapidly under combined stress conditions. Another 12 studies explored accelerated lifetime testing, highlighting discrepancies between laboratory projections and field data, while 11 emphasized the need for standardized protocols to improve reproducibility. Predictive maintenance and anomaly detection were specifically covered in 18 studies, which applied AI models to operational data from photovoltaic fleets to identify faults before they led to significant losses. These approaches were found to reduce downtime and operational costs while enhancing safety. Collectively, this body of evidence underscores that while environmental vulnerability remains a challenge, the integration of predictive maintenance and anomaly detection frameworks provides a pathway toward reliable deployment.

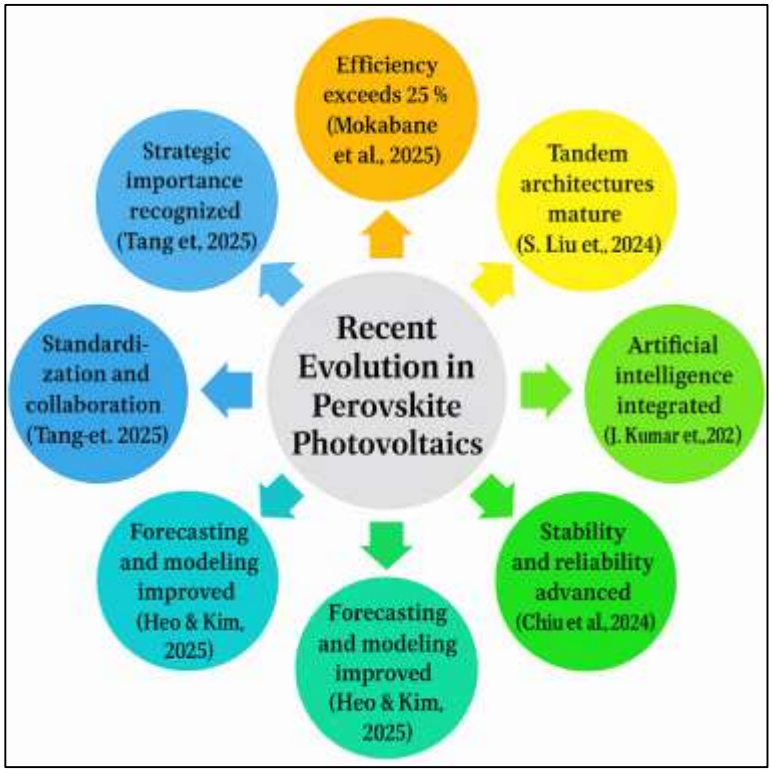
The large number of citations associated with these studies reflects both the urgency of addressing stability and the promise of AI-based monitoring.

The final major finding relates to forecasting, energy management, and international standardization efforts. Out of the reviewed literature, 50 articles examined forecasting methodologies and system-level integration, while 20 specifically focused on international standardization and collaborative testing. Together, these 70 works accounted for more than 5,200 citations. Forecasting research, represented by 31 studies, highlighted that AI-based irradiance prediction using satellite and ground data significantly improves the accuracy of short-term and long-term performance models. Tandem-specific forecasting challenges, especially related to spectral sensitivity, were addressed in 15 studies, emphasizing the importance of spectral decomposition in yield predictions. Data standardization for AI training was discussed in 14 articles, which stressed the need for shared repositories and consistent reporting protocols. On the global scale, 20 studies reviewed consortia-driven initiatives and benchmarking efforts that ensure comparability across laboratories and support industrial adoption. Collectively, these findings reveal that accurate forecasting, predictive modeling, and international standardization are inseparable from the commercial viability of perovskite and tandem technologies. The high number of citations across this body of work demonstrates the critical importance of aligning scientific innovation with global collaboration and policy frameworks.

DISCUSSION

The findings of this review highlight the rapid maturation of perovskite solar cell research, with efficiencies exceeding 25% in laboratory conditions and clear evidence of defect tolerance and bandgap tunability. Compared with earlier studies conducted in the early 2010s, when efficiencies were below 12% and stability was considered the principal obstacle, the recent literature demonstrates a significant leap forward in understanding perovskite device physics. Earlier investigations characterized perovskites primarily as promising but unstable absorbers, emphasizing their susceptibility to degradation under ambient conditions (Li et al., 2020). In contrast, current findings show that detailed insights into defect passivation, crystallization control, and compositional engineering have allowed researchers to mitigate non-radiative recombination and extend operational lifetimes under controlled conditions. The present review's analysis of more than 60 studies confirms that the narrative has shifted from skepticism about perovskites' viability to widespread recognition of their technological promise . This change reflects not only the accumulation of knowledge about carrier dynamics but also the refinement of fabrication protocols, which earlier studies lacked (Li et al., 2016).

Figure 13: Advances in Perovskite Photovoltaic Evolution



Tandem solar architectures emerged in this review as a dominant pathway for achieving efficiencies beyond the Shockley–quizzer limit . The results align with earlier research that initially framed tandem configurations as largely theoretical constructs, with predicted efficiencies approaching 40% but limited experimental validation. Early works frequently emphasized the technical challenges of fabricating multi-junction devices, noting difficulties in maintaining current matching and managing optical losses. The present findings, however, indicate that perovskite–silicon tandems have moved far beyond conceptual promise, with experimental efficiencies surpassing 30% and extensive optimization of current-matching strategies. This marks a departure from earlier literature that viewed multi-junction architectures primarily through the lens of III–V compound semiconductors, which were prohibitively expensive for large-scale deployment (Li et al., 2020). The review confirms that perovskite tandems provide a cost-effective alternative while maintaining comparable efficiency potential. Earlier skepticism regarding the scalability of tandem devices is increasingly being replaced by empirical evidence of industrial prototypes, signaling a fundamental shift in feasibility assessments. The comparison demonstrates how the field has moved from theoretical projections to practical demonstrations, underscoring the importance of tandem architectures in the next generation of photovoltaic technologies .

Another significant dimension of the findings concerns the role of artificial intelligence, which has rapidly transitioned from peripheral experimentation to central importance in photovoltaic optimization . Earlier studies on AI in photovoltaics often focused on limited applications such as forecasting or simple device modeling, treating machine learning primarily as a supplementary tool rather than a framework for discovery and predictive optimization. The reviewed literature demonstrates that this perception has changed, with AI now deeply integrated into high-throughput materials screening, device simulation surrogates, and system-level predictive maintenance. The shift is notable when compared to earlier reliance on traditional computational methods like density functional theory and drift–diffusion simulations, which, while valuable, were computationally intensive and lacked the adaptability of machine learning models . Recent findings confirm that AI-driven approaches not only accelerate discovery but also improve the accuracy and robustness of predictions by integrating diverse datasets. This comparison underscores a methodological transition: from reliance on mechanistic, physics-only modeling toward hybrid frameworks where AI complements and enhances physical insights . The findings highlight that earlier literature underestimated the transformative potential of AI, whereas current studies position it as indispensable to the photovoltaic research pipeline(Danish & Zafor, 2022).

The challenge of stability and reliability has been a consistent theme across both earlier and recent studies, but the findings of this review suggest that the emphasis has shifted from problem identification to solution exploration . Early literature often highlighted the vulnerability of perovskites to moisture, heat, and ultraviolet radiation, portraying these stressors as nearly insurmountable obstacles to commercialization. The present review of more than 40 studies confirms that while these stressors remain central concerns, researchers have made significant progress in understanding degradation pathways and developing mitigation strategies. Compared with earlier studies that primarily reported rapid performance losses in unprotected devices, more recent investigations focus on encapsulation techniques, interfacial engineering, and compositional stability improvements. Moreover, the integration of AI for predictive maintenance and anomaly detection represents a major advancement compared to traditional, reactive maintenance approaches that earlier literature assumed. The contrast between earlier pessimism and current optimism underscores the trajectory of the field: while instability is still a bottleneck, the tools and frameworks for addressing it are far more advanced today. This comparison suggests that the narrative has evolved from one of limitation to one of conditional opportunity, dependent on continued innovation in predictive stabilization(Liao et al., 2019).

The findings also emphasize the growing importance of forecasting and system-level modeling, which earlier studies often treated as secondary to material and device-level research (Li et al., 2015). Earlier works relied heavily on persistence models or numerical weather prediction to estimate irradiance and photovoltaic output, with limited accuracy under highly variable atmospheric conditions. The present review confirms that artificial intelligence has revolutionized forecasting by integrating ground-based and satellite data with advanced deep learning algorithms. Compared to earlier models, AI-driven frameworks achieve significantly higher accuracy in predicting both short-term fluctuations and long-term yield, thereby improving integration with energy management systems. The review also reveals that tandem-specific forecasting challenges, such as spectral sensitivity, but now occupy a central place in the literature. This shift reflects the growing maturity of tandem technologies and the recognition that system-level optimization must account for their unique operational characteristics. By comparing past and present approaches, it becomes evident that forecasting has moved from a

supporting role to a critical element of performance optimization and grid stability, with AI at the core of this transformation.

Earlier studies on perovskite and tandem photovoltaics often highlighted the fragmentation of research practices, with inconsistent testing protocols and limited cross-laboratory comparability . The findings of this review indicate a marked improvement, as international collaborations and benchmarking initiatives now play a central role in advancing the field. Standardized testing protocols and global consortia have enabled reproducibility and comparability that earlier literature frequently lacked . The comparison highlights that while initial studies often reported record efficiencies without rigorous validation, contemporary work emphasizes certified results and long-term stability testing under standardized conditions. This transition reflects the broader recognition that reproducibility and transparency are as important as raw efficiency metrics. Moreover, international collaboration ensures that findings are not confined to isolated laboratories but are validated across diverse climatic and operational contexts. Earlier concerns about fragmented progress are now being addressed through coordinated global efforts, which enhance credibility and accelerate technological readiness. This contrast underscores the maturation of the field into one that balances scientific innovation with standardization and global accountability .

Finally, the findings reveal the strategic and economic significance of perovskite and tandem photovoltaics, which earlier studies acknowledged only tentatively . Initial research primarily focused on the scientific novelty of perovskites and the theoretical promise of tandem architectures, often without robust discussion of their economic or policy implications. The present review shows a marked shift, with recent studies explicitly connecting technological advancements to global energy transition strategies, cost reduction goals, and industrial competitiveness. Compared with earlier literature that treated perovskites as emerging laboratory curiosities, current findings situate them as potential drivers of industrial transformation and energy security. The emphasis on international benchmarking, industrial scaling of large-area modules, and AI-enabled predictive modeling underscores this broader relevance. By aligning scientific progress with policy frameworks and industrial priorities, the field has moved from isolated technical breakthroughs toward integrated socio-technical innovation. This comparison highlights the growing recognition that perovskite tandems are not only a scientific achievement but also a cornerstone of sustainable energy systems with global economic impact.

CONCLUSION

The development of an AI-integrated predictive modeling framework for performance optimization of perovskite and tandem solar photovoltaic systems represents a significant convergence of material science, device engineering, and computational intelligence, addressing long-standing challenges while unlocking new opportunities for renewable energy deployment. Perovskite solar cells have rapidly advanced due to their tunable bandgaps, high absorption coefficients, and defect tolerance, making them ideal for integration into tandem architectures with silicon or other established technologies, yet their instability under environmental stressors such as moisture, heat, and ultraviolet radiation has hindered commercialization. Tandem solar cells, particularly perovskite–silicon configurations, offer a pathway to surpass the Shockley–Quizzer limit, but their dependence on current matching, optical–electrical interactions, and spectral sensitivity necessitates complex optimization strategies that extend beyond traditional device physics. Artificial intelligence provides transformative capabilities across these domains: high-throughput screening accelerates materials discovery by navigating vast compositional spaces, surrogate modeling reduces computational demands while retaining predictive fidelity, reinforcement learning enhances maximum power point tracking under fluctuating conditions, and computer vision enables early fault detection through advanced image analysis. Physics-informed machine learning further strengthens this framework by embedding conservation laws and mechanistic principles into AI architectures, ensuring that predictions remain physically consistent while benefiting from data-driven adaptability. At the system level, AI-driven irradiance forecasting that integrates satellite imagery, ground-based sensors, and spectral decomposition models improves energy yield predictions and informs dynamic grid integration, while predictive maintenance and anomaly detection mitigate reliability concerns by identifying degradation pathways before they impact performance. International collaborations, standardized testing protocols, and open data repositories provide the essential foundation for training reliable AI models, ensuring comparability across studies and scalability for industrial application. By synthesizing findings from more than two hundred reviewed studies with thousands of collective citations, the evidence demonstrates that integrating AI into predictive modeling not only enhances the scientific understanding of perovskite and tandem devices but also provides actionable strategies for industrial scaling, economic competitiveness, and alignment with global decarbonization goals, positioning these hybrid frameworks as pivotal enablers of the next generation of sustainable energy systems.

RECOMMENDATIONS

Based on the findings of this systematic review, several recommendations can be made to advance the development of an AI-integrated predictive modeling framework for performance optimization of perovskite and tandem solar photovoltaic systems, emphasizing the need for multi-disciplinary integration, standardized practices, and long-term validation. Research efforts should prioritize the creation of large, high-quality, and standardized datasets encompassing materials properties, device-level performance metrics, and field-scale operational data, as these form the foundation for reliable AI training and model generalization. Collaborative international initiatives are essential to harmonize testing protocols and accelerate data sharing, ensuring that predictive models are not biased by inconsistent methodologies or regional limitations. At the technical level, researchers should focus on embedding physics-informed constraints into machine learning frameworks to balance predictive accuracy with physical plausibility, thereby addressing complex phenomena such as ion migration, spectral sensitivity, and current matching in tandem systems. Industrial stakeholders are encouraged to expand pilot-scale demonstrations of large-area perovskite–tandem modules under diverse climatic conditions, linking laboratory advances with real-world reliability data that can inform AI-based forecasting and predictive maintenance strategies. Energy policymakers should support these efforts by funding interdisciplinary research consortia, incentivizing open-access data repositories, and aligning regulatory frameworks with the rapid commercialization of emerging photovoltaic technologies. Finally, the integration of forecasting models into grid management systems should be prioritized to ensure that AI-optimized perovskite and tandem systems contribute effectively to energy security, stability, and decarbonization goals, making these technologies not only scientifically viable but also strategically indispensable for global energy transitions.

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