

Application of Photoelectric Effect and Electron Diffraction for Optimizing the Efficiency of Perovskite Solar Cells: A Literature Review

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Abstract

As the next generation of photovoltaic devices, perovskite solar cells have a lot of promise. But material deterioration and instability present a serious problem. This article reviews how the photoelectric effect and electron diffraction can help improve device performance through a PRISMA-based Systematic Literature Review. The review looks at fifteen studies that were published between 2020 and 2025, with an emphasis on energy conversion processes, structural stability, and characterization techniques. The synthesis shows that electron-based methods are essential for detecting crystal defects, halide segregation, and degradation behavior under operando conditions. These methods include in situ TEM, EBSD, four-dimensional STEM, SAED, and TEM. The results highlight how crucial it is to manage microstructure, lessen ion segregation, and uphold standard characterization procedures in order to increase stability and effectiveness. Since no previous work has fully integrated photovoltaic mechanisms with electron diffraction in a single framework, this review addresses a clear research gap and encourages multimodal operando approaches with better film growth control.

Keywords: Material Stability, Photoelectric Effect, Electron Diffraction, Transmission Electron Microscopy (TEM), Perovskite Solar Cell (PSC).

INTRODUCTION

Ensuring access to sustainable energy is one of the major challenges of the twenty-first century (Falcone, 2023). Environmental preservation and resource conservation are global priorities because excessive energy use exacerbates pollution, acid rain, and global warming (Isabelle dos Santos et al., 2024). Although fossil fuels continue to supply more than 80% of the world's energy and significantly contribute to greenhouse gas emissions, growing industrialization and population growth further strain economic and environmental systems (Dastgeer et al., 2024).

Perovskite solar cells are a promising third-generation photovoltaic technology (Wu et al., 2021). Early research developed scalable deposition methods like spray coating, doctor-blade, and slot-die (Shi & Jayatissa, 2018), which set the stage for quick increases in efficiency. Building on this basis, power conversion efficiency increased from about 3% to over 25% between 2020 and 2025 (Khatoun et al., 2023). Long-term stability is a major area of current research, though, as it still lags behind efficiency gains.

The photoelectric effect in the perovskite layer, where light absorption produces electron-hole pairs that transform into electrical current, is what drives PSC efficiency. Device performance is further improved by superior optoelectronic characteristics, such as strong absorption, long diffusion lengths, and high charge mobility (Roy et al., 2022). To increase productivity, it is essential to comprehend this mechanism.

Device stability is significantly impacted by the perovskite crystal's quality. Grain shape, crystal orientation, and structural defects all have a significant effect on long-term operation (L. Huang et al., 2023). Defect distribution and phase behavior are revealed by electron diffraction techniques like SAED and TEM, which shed light on these characteristics (Zhang et al., 2023). According to in situ TEM research, degradation entails phase transitions and structural damage that lower stability and efficiency (B. Li et al., 2024). Electron diffraction therefore facilitates both structural optimization and material characterization.

As lead-free substitutes, tin-based perovskites are another sustainable route. Methods like nucleation engineering and two- and three-dimensional heterostructures have produced efficiencies of about 16.65 percent and stability of more than 1500 hours without encapsulation (He et al., 2025). Additionally, interfacial engineering with self-assembled monolayers can improve device durability by reducing nonradiative recombination and increasing charge extraction (Tian & Zhang, 2024).

In light of these advancements, this review analyzes the photoelectric effect as the basis for energy conversion and looks at how electron diffraction helps with PSC optimization. This study assesses methods that improve stability and efficiency through electron-based characterization and basic mechanism understanding, with a focus on recent literature from the last ten years. Since no systematic review has yet combined these two components into a single analytical framework, this work fills a critical research gap and provides a basis for more targeted future research.

RESEARCH METHODS

The Systematic Literature Review for this study adhered to PRISMA guidelines. (Page et al., 2021). Using the keywords perovskite solar cell, photoelectric effect, electron diffraction, TEM, SAED, EBSD, and efficiency improvement, a thorough search was carried out through Scopus, ScienceDirect, DOAJ, and Google Scholar, restricted to publications from 2020 to 2025. Journal articles and conference papers pertaining to PSCs, photoelectric mechanisms, and electron diffraction-based material analysis were included; duplicates, unrelated studies, and unavailable full texts were not. The goals, approaches, outcomes, and contributions to PSC optimization of the eligible articles were further scrutinized. Descriptive and qualitative analysis through thematic grouping, cross-study comparison, and integration of findings were all part of the synthesis. The accompanying PRISMA flowchart summarizes each step, from identification to final inclusion.

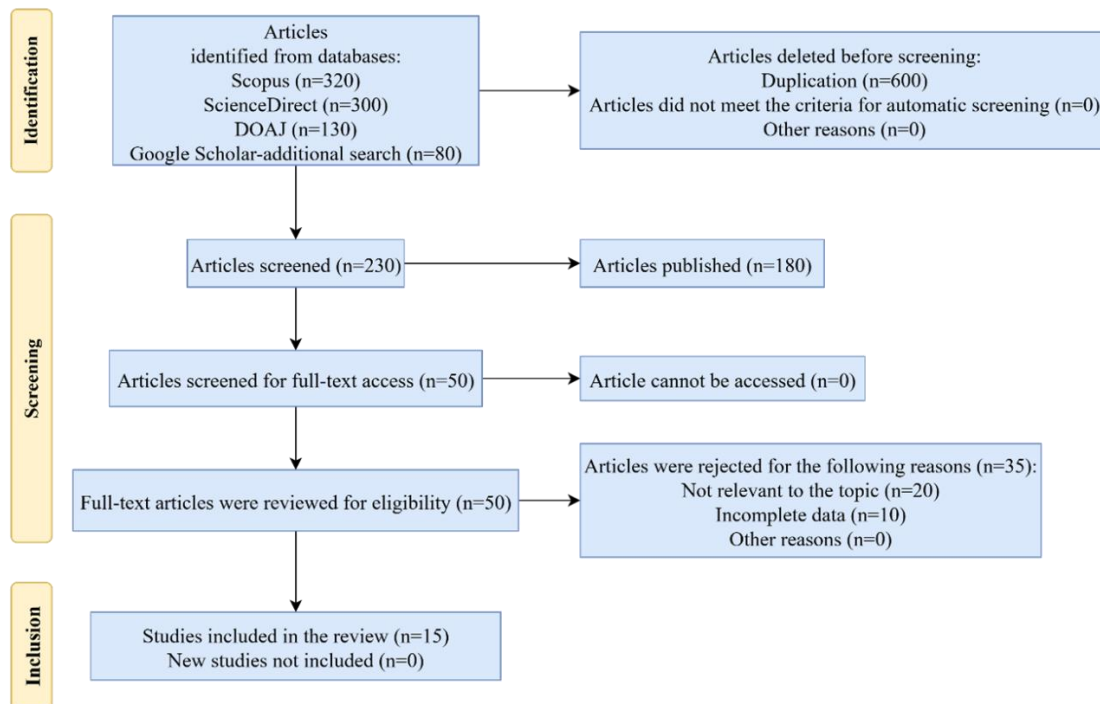


Figure 1. PRISMA Flow Chart

RESULTS AND DISCUSSION

PSC Theoretical Basis

An ABX_3 perovskite crystal structure, in which X is a halide and A and B are either organic or inorganic cations, is used in perovskite solar cells. Strong light absorption and effective charge transport provided by this structure enable energy conversion via the photoelectric effect (Suresh Kumar & Chandra Babu Naidu, 2021). Figure 2 shows the fundamental PSC architecture, with the perovskite layer acting as the main absorber and the electron and hole transport layers directing charges to the electrodes.

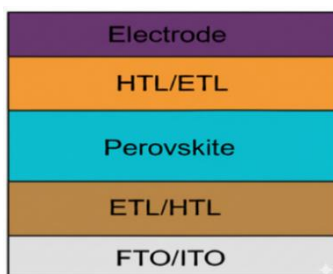


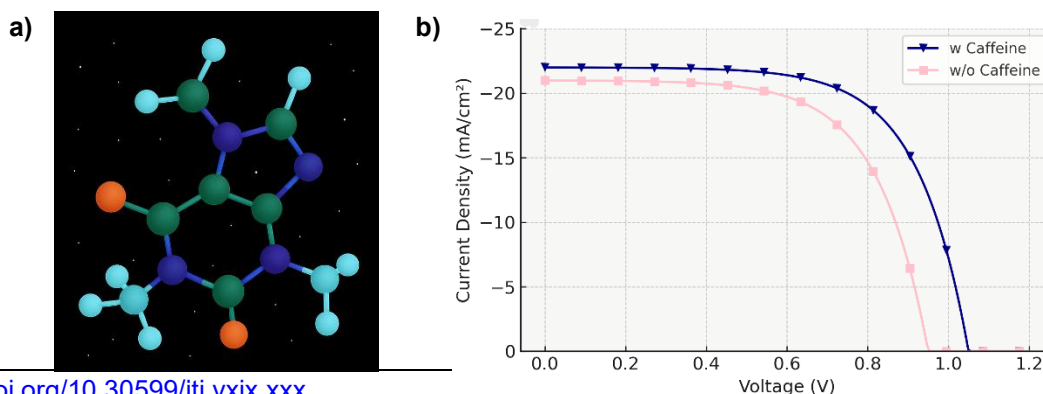
Figure 2. The fundamental structure of a perovskite solar cell (PSC) (Osman et al., 2021)

The photoelectric process begins with photon absorption and proceeds to electron-hole pair formation, charge separation, and transport. These processes are influenced by bandgap, absorption coefficient, and crystal quality (Miah et al., 2024). While crystal defects produce trap states that lower voltage and current, proper cation and halide combinations increase mobility and decrease recombination (Zhang et al., 2023). Cation substitution and defect passivation aid in preserving performance in challenging circumstances (Seshaiah & Kim, 2024).

Phase stability, diffusion length, and charge mobility are important optoelectronic factors. Stability is increased and recombination is suppressed by bandgap grading, halide substitution, and enhanced crystallinity (W. Cao et al., 2022; Y. Cao et al., 2025). High device efficiency and film uniformity are also determined by fabrication control, which includes interface engineering, annealing, and solvent selection (Mokabane et al., 2025).

Perovskite Solar Cells' Main Obstacles

Despite significant efficiency gains, PSCs' poor long-term stability under humidity, oxygen, heat, and continuous illumination continues to be the main obstacle to commercialization (Sharshir et al., 2025). Moisture resistance is a major focus of material engineering because moisture and oxygen speed up metastable phase transitions and crystal breakdown, which lowers photovoltaic performance. Internal electric field distortion, interfacial charge accumulation, and both reversible and irreversible degradation are the results of ion migration involving cations and halide ions, which ultimately decreases operational stability and increases hysteresis in the current–voltage (J–V) curve (R. Li et al., 2024). Figure 3 shows this hysteresis behavior, which is directly related to ion migration.



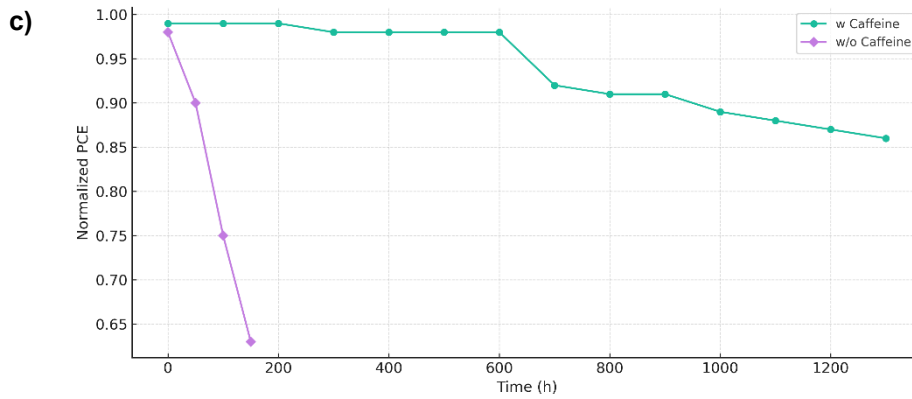


Figure 3. Perovskite Solar Cell's J-V Curve Illustrating the Hysteresis Phenomenon (Khatoun et al., 2023).

Ion migration reduces PSC operational stability while increasing hysteresis. The following drift diffusion equation can be used to explain ion migration:

$$Q_I = \epsilon_s E_{bi} + \epsilon_s E \left[\exp\left(-\frac{q\mu_I Nt}{\epsilon_s}\right) - 1 \right] \quad (1)$$

The equation, where ϵ_s , q , μ_I , N , and t stand for permittivity, electron charge, ion mobility, ion concentration, and time, describes ion charge accumulation (Q_I) in the perovskite layer under internal (E_{bi}) and external electric fields (E). Time-dependent ion accumulation that causes hysteresis and lowers PSC stability is reflected in the exponential term (R. Li et al., 2024).

Water-induced degradation also speeds up the dissociation of perovskite into non-photoconductive phases (Q. Li et al., 2021). Atomic-scale studies have shown that water molecules mediate nanoscale degradation pathways, highlighting the importance of protective layers and humidity control during fabrication (B. Chen et al., 2022; Tang et al., 2024)

Another crucial problem is thermal instability because high temperatures can cause phase transitions and crystal defects. Under thermal stress, structural degradation dynamics are revealed by in-situ TEM observations, which reduce photovoltaic performance (Seo et al., 2020). Figure 4 illustrates this thermally induced degradation at grain boundaries.

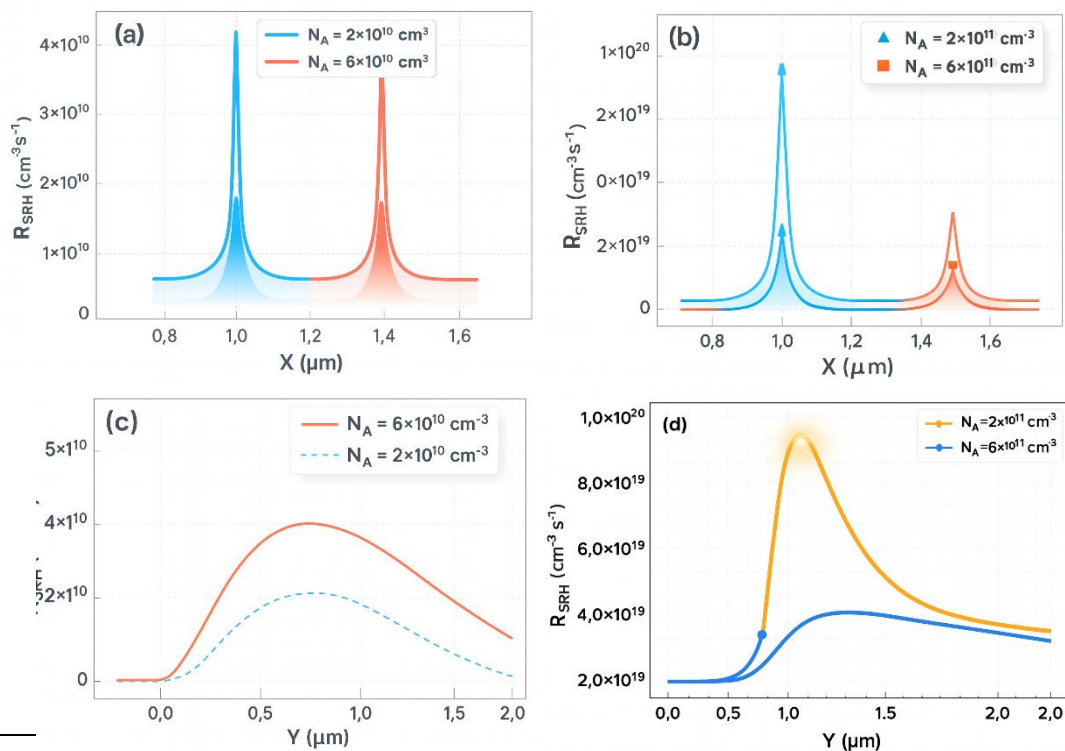


Figure 4. Crystal Recombination and Degradation Visualization at Grain Boundaries (Urbaniak et al., 2025)

Defects at grain boundaries accelerate charge recombination and device degradation. Grain morphology and void formation are significantly influenced by perovskite film quality and fabrication parameters such as humidity, solvent selection, and annealing conditions (Mesquita et al., 2020). Atomic vacancies, deep traps, and grain-boundary defects serve as non-radiative recombination sites that reduce J_{sc} and V_{oc} (Kaiser et al., 2022). The recombination mechanism is explained by the Shockley-Read-Hall (SRH) model:

$$-\frac{dn}{dt} = k_1n + k_2n^2 + k_3n^3 \quad (2)$$

where k_2 represents band-to-band radiative recombination, k_3 represents Auger recombination, and k_1 represents the non-radiative recombination rate (SRH) (Guo et al., 2024). It has been demonstrated that increasing grain size suppresses these flaws and enhances stability and efficiency (Urbaniak et al., 2025).

Although lead-free tin-based PSCs have also been studied, Sn^{2+} easily oxidizes to Sn^{4+} , which lowers performance and increases defects (Liu et al., 2023). Stabilization typically requires chemical treatments and the addition of antioxidants. Overall, a multimodal approach that incorporates interface engineering, passivating additives, and crystallization control yields the greatest improvements in defect mitigation (Jiang et al., 2025). Additionally, field durability tests demonstrate how radiation, temperature, humidity, and ion migration interact to cause degradation in the real world, highlighting the necessity of standardized stability metrics (Tayagaki et al., 2024).

Therefore, creating moisture-resistant materials, creating efficient encapsulation, and preserving fabrication consistency are all necessary to increase PSC durability. To lower trap density and attain long-term device stability, material engineering must be integrated with nanoscale characterization instruments like TEM, SAED, and in situ diagnostics (Yantara & Mathews, 2024).

The Role of Electron Characterization

1. Transmission Electron Microscopy (TEM)

Transmission electron microscopy (TEM) is an essential technique for characterizing perovskite halides, particularly for identifying structural defects that act as sites for charge recombination (Yao et al., 2023). Defects that reduce energy conversion efficiency and accelerate nonradiative recombination include dislocations, grain boundaries, and point defects. To minimize electron-beam damage and obtain precise observations of atomic structure and grain morphology, low-dose TEM is necessary (Yan et al., 2025). The TEM setup for perovskite characterization is shown in Figure 5.

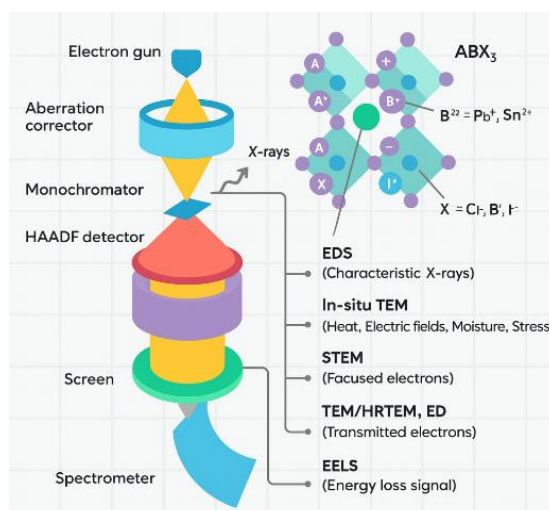


Figure 5. Diagrammatic Representation of the TEM Configuration for Halide Perovskite Analysis (Yao et al., 2023)

Low-dose imaging allows for the precise observation of structural defects without causing material damage. To analyze surfaces and interfaces without adding artifacts, high-resolution TEM (HRTEM) and STEM can be used in conjunction with methods like correlative TEM and cryo-TEM (Y. Zhu et al., 2020). Additionally, TEM offers vital information about the interactions between the perovskite and transport layer that control charge extraction (B. Li et al., 2024). Further research reveals a correlation between performance degradation and crystallographic heterogeneity and nanoscale grain distribution. In order to comprehend long-term PSC degradation mechanisms, TEM functions as a diagnostic and predictive tool (C. Zhu et al., 2023).

2. Selected Area Electron Diffraction (SAED)

Local perovskite crystal phases can be identified and structural alterations brought on by heat or humidity can be assessed using Selected Area Electron Diffraction (SAED) (Dhanalaxmi et al., 2025). Its diffraction patterns reveal interplanar spacing and structural order while accurately detecting halide segregation and minor degradation phases like PbI_2 at the nanoscale (W. Cao et al., 2022). Additionally, SAED monitors phase changes that occur during fabrication or thermal treatment procedures (Hun et al., 2025). It records lattice fluctuations that could affect charge mobility anisotropy when paired with pixelated detectors or 4D-STEM (Fan et al., 2025). In order to support PSC degradation analysis and optimization, SAED is a crucial method that connects atomic-scale structure to macroscopic photoelectric behavior (El Bachraoui et al., 2022).

3. In-Situ TEM

Real-time monitoring of perovskite structural evolution under operando conditions like heating, electrical bias, humidity, and illumination is made possible by in-situ TEM (Seo et al., 2020). According to Darsan & Pandikumar (2024), thermal treatment can cause halide and metal ion migration, which can result in voids and degradation phases that hasten performance loss. The interaction between water molecules and the perovskite surface, which encourages weathering and defect formation, is further revealed by liquid-phase in-situ TEM. It provides quantitative understanding of photoelectric fluctuations and hysteresis by tracking Br^- and I^- segregation at the nanoscale when combined with strain mapping and 4D-STEM (Kleibert et al., 2025). Because it assesses stabilization techniques like encapsulation and passivation by directly visualizing microstructural responses under realistic conditions, in-situ TEM is essential for developing effective degradation-mitigation strategies for PSC (Kennedy et al., 2025).

4. Backscatter Diffraction (EBSD)

Although their application in perovskites is still restricted because of beam sensitivity, low-dose Electron Backscatter Diffraction (EBSD) and Transmission Kikuchi Diffraction (TKD) present new opportunities for crystal orientation mapping (Y. Wang et al., 2025). Micron to sub-micron grain distributions that frequently serve as recombination centers are identified by EBSD (Kennedy et al., 2025). These methods allow for precise strain and heterogeneity mapping using sophisticated detectors when paired with 4D-STEM (Zambon et al., 2023). Designing films with better charge transport is aided by an understanding of crystal texture and grain orientation. Integrating EBSD/TKD with TEM and 4D-STEM is regarded as a promising multimodal approach, though it is still in its early stages of development (Y. Wang et al., 2025).

Efficiency and Stability Optimization Strategy

1. Interface Engineering

One important tactic for enhancing charge extraction and reducing non-radiative recombination in PSCs is interface engineering. Self-assembled monolayers (SAMs), passivating molecules, and buffer interlayers are examples of functional thin layers that have been demonstrated to enhance energy level alignment, lower surface trap density, and boost resistance to oxygen and moisture (Heo et al., 2022). Large-scale production of homogeneous films is made possible by the application of SAMs on the hole-transport layer (HTL)/perovskite or perovskite/electrode interface, which successfully lowers surface defects and suppresses V_{oc} loss (Fu et al., 2025).

Furthermore, the device's service life can be increased by adding an ion barrier layer or selective transport layer (Du et al., 2025; Z. Wang et al., 2025). Devices with high power conversion efficiency

(PCE) and improved performance retention under ambient humidity and temperature conditions are produced by combining interface engineering with chemical additives, both organic and inorganic (Hossain Howlader et al., 2024). Another method for achieving bandgap optimization is graded heterostructure engineering, which is expressed mathematically as:

$$E_g(x) = \Delta E_g \exp \left[- \left(\frac{10^9 \sqrt{2\pi x}}{d_g} \right)^2 \right] + E_g \quad (3)$$

With ΔE_g as the maximum variation and "graded depth" as the gradient depth, this equation demonstrates how the bandgap profile varies continuously with position (Y. Cao et al., 2025).

2. 2D/3D Structure

Efficiency and stability are balanced by 2D/3D heterostructures. Ruddlesden–Popper-type 2D layers on surfaces or grain boundaries can create energy barriers that more effectively direct charge toward electrodes, prevent water penetration, and suppress recombination at grain boundaries (X. Li et al., 2023). Figure 6 illustrates the idea of 2D/3D heterostructure architecture, which is frequently employed in perovskite solar cells (PSCs).

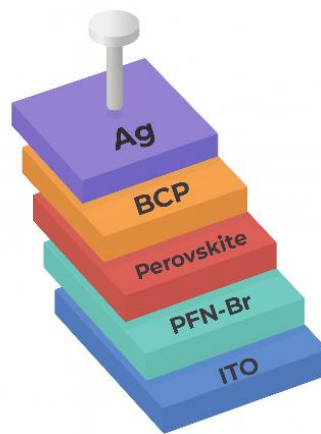


Figure 6. 2D/3D Heterostructure Schematic (X. Li et al., 2023).

In long-term testing, including in large-scale modules, engineered 2D/3D structures via epitaxial control or nucleation have been demonstrated to decrease trap density, slow ion migration, and enhance thermal stability and PCE retention (Y. Chen et al., 2025). Figure 7 illustrates how the interface band alignment affects the charge transport dynamics in 2D/3D heterostructures.

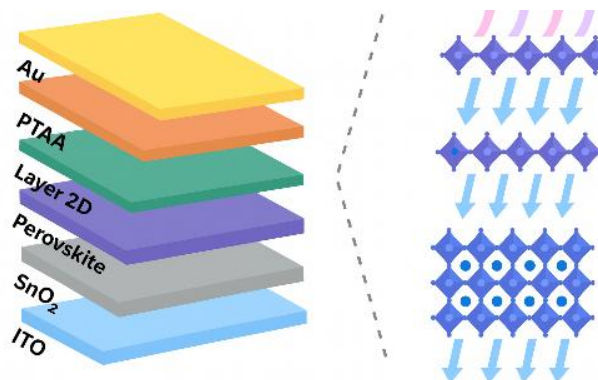


Figure 7. Diagram of Charge Transport Dynamics in a 2D/3D Heterostructure (X. Li et al., 2023).

This plan demonstrates that the 2D layer functions as an energy barrier that inhibits recombination while more effectively directing carriers, supporting increased device stability and efficiency.

It has been reported that using synthesis methods and solvent formulations that encourage large grain growth and the creation of 2D/3D heterostructures can boost productivity while lowering the rate of degradation in thermal and humidity tests (G. Huang et al., 2025). Translating laboratory efficiency into field performance currently focuses on mapping the relationship between 2D/3D architecture, load dynamics, and degradation resistance (Liang et al., 2024).

3. Material Substitution

An alternative to dealing with the problem of Pb toxicity is the development of tin-based perovskite (Sn-based). The oxidation of $\text{Sn}^{2+} \rightarrow \text{Sn}^{4+}$, which raises defect density, lowers V_{oc} , and diminishes stability, is the primary obstacle. Interface engineering, antioxidant additive addition, and A/B-site composition tuning have all been used in stabilization efforts (Mahmoudi et al., 2025). In both humid and inert environments, molecular passivation in conjunction with a functional interface layer has increased PCE to competitive levels and extended performance retention (Ayaydah et al., 2023; Subudhi et al., 2025).

Additionally, a 2D protective layer applied to a 3D/2D heterostructure effectively prevents oxidation and ion migration, promoting long-term stability (Ouyang et al., 2025). The 3D/2D heterojunction structure with a 2D protective layer is shown in Figure 8.

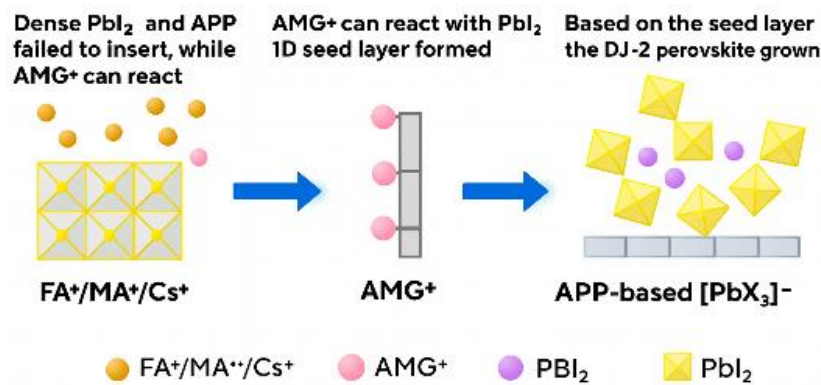


Figure 8. 3D/2D Perovskite Heterojunction Configuration Diagram (Ouyang et al., 2025).

All things considered, the most promising approach to achieving effective, stable, and ecologically friendly PSCs is the combination of interface engineering, 2D/3D heterostructures, and material substitution, supported by chemical passivation and fabrication control (Abdelghafar et al., 2025).

Synthesis Literature Findings

Table 1. Summary of Studies Related to the Photoelectric Effect and Electron Characterization in PSC

No	References	Material/Composition	Characterization Technique	Main Focus	PCE (%)	Key Findings
1	(Yao et al., 2023)	Perovskites with halides	Review of low-dose TEM	Imaging with on-destructive beams	-	It provides a low-dose protocol to reduce artifacts and is a standard for characterizing electron-sensitive PSCs.
2	(Hao & Cai, 2025)	Nanocrystals of halide perovskite	In-situ TEM (humid, water vapor)	Examining phase transition, grain growth, and degradation in a water vapor	-	Moisture accelerates deterioration and reduces crystal quality at grain boundaries.

3	(Fan et al., 2025)	<i>I/Br mixed-halide</i>	4D-STEM functionality	environment Dynamics of halide segregation	-	Real-time Br ⁻ /I ⁻ segregation; hysteresis and Voc decrease are correlated.
4	(Dhanalaxmi et al., 2025)	<i>Various PSC</i>	TEM, SAED, operando	Characterization & stability roadmap	-	Integrative review with a focus on characterization's role in PSC scaling.
5	(Kovalenko et al., 2025)	<i>Oriented 2D platelets</i>	TKD / EBSD	Crystal orientation & texture	18.2	Anisotropic transport and Jsc are improved by controlled crystal orientation.
6	(S. Chen et al., 2020)	<i>Hybrid PSC</i>	TEM/HRTEM (review)	Imaging artifacts	-	The conventional TEM technique for hybrid perovskites.
7	(Seo et al., 2020)	<i>MAPbI₃, CsPbI₃</i>	In-situ heating TEM	Ion migration & thermal degradation	19.5	PCE decreased from 19.5% to less than 10% due to the formation of PbI ₂ during heating.
8	(An et al., 2021)	<i>Polycrystalline PSC</i>	Correlative TEM + optical	Grain boundary & recombination	21.1	Recombination centers due to small grains reduce Voc and FF.
9	(Shen et al., 2023)	<i>PSC with passivators</i>	TEM + spectroscopy	Defect reduction	23.0	Passivation decreases trap states, and longer stability is supported by TEM data.
10	(Duan et al., 2023)	<i>PSC under PSC with passivators illumination</i>	In-situ TEM (light bias)	Structural response when light is biased	22.3	Hysteresis is decreased by direct observation of ion dynamics during operation.
11	(N. Li et al., 2025)	<i>Berbagai PSC (review)</i>	In-situ TEM	Methodological challenges	-	Artifacts and operando cell requirements are discussed.
12	(Fan et al., 2025)	<i>Mixed-halide PSC</i>	Cryo-STEM + 4D-STEM	Photoinduced segregation	20.7	Ion segregation is demonstrated to have an impact on Voc, and cryo stabilizes the metastable phase.
13	(Pfeifer et al., 2025)	<i>PSC with TEMPO</i>	TEM + device testing	Grain boundary passivation	24.5	TEMPO passivation improves stability to >1000 hours and raises PCE by up to 24.5%.
14	(Z. Li et al., 2023)	<i>Mixed-halide wide-bandgap</i>	In-situ TEM	Blocking layer & stability	20.8	By suppressing halide segregation, the blocking layer raises Voc.
15	(B. Li et al., 2024)	<i>Broad perovskites</i>	TEM/SAED/XRD (review)	Degradation mechanism	-	Thorough analysis and suggestions for characterization strategies.

Research on perovskite solar cells (PSCs) has moved from improving power conversion efficiency (PCE) to a mechanistic understanding of the impact of microstructure on performance, according to a review of 15 recent articles published between 2020 and 2025. Low-dose/cryo-TEM, in-situ TEM, 4D-STEM, and EBSD/TKD are examples of electron-based characterization techniques that have proven

crucial for illuminating the degradation dynamics, ion migration, halide segregation, and crystal orientation that dictate photovoltaic behavior.

There were three primary patterns found. First, film growth and passivation engineering are necessary because grain boundaries serve as recombination centers. Second, halide segregation lowers Voc and causes hysteresis, which can be managed by alloying or blocking layers. Third, the standardization of low-dose, cryo, and operando protocols is crucial because different characterization approaches continue to yield inconsistent data. These results validate that a strategic approach for PSC development is to combine advanced characterization techniques with material engineering strategies.

There are still some discrepancies despite the general consensus. For instance, some research emphasizes thermal or structural degradation even in the dark (Seo et al., 2020; Urbaniak et al., 2025), while other research primarily links J–V hysteresis to light-induced halide migration (Duan et al., 2023; Fan et al., 2025). This implies that a unified stability model is still elusive and that dominant degradation pathways may be dependent on external stressors.

Research Implications

A review of the literature supports a number of significant implications for the future of PSC research. First, because variations in electron dose, temperature, and environmental conditions in TEM studies frequently produce data that is challenging to replicate, standardization of electron characterization methodologies is crucial (S. Chen et al., 2020). It has been demonstrated that low-dose and cryo-TEM protocols are more representative and could become the norm (Yao et al., 2023). Second, there is growing promise in the integration of operando approaches. Liquid-phase in-situ TEM demonstrates rapid degradation by water (Hao & Cai, 2025), in-situ TEM reveals the formation of PbI₂ and voids due to heating (Seo et al., 2020), and LI2ST successfully visualizes ion migration under light bias directly related to hysteresis in the J–V curve (Duan et al., 2023).

Third, optimization relies heavily on microstructure control. While uniform crystal orientation enhances anisotropic charge transport and PCE (Kovalenko et al., 2025), small grains are identified as recombination centers that lower Voc and fill factor (An et al., 2021). Fourth, operando 4D-STEM has shown that halide segregation decreases Voc and deteriorates stability (Fan et al., 2025). Partial solutions are provided by blocking layers or compositional engineering. Fifth, the trend toward multimodal methods, like combining TEM with synchrotron nano-XRD or soft X-ray microscopy, improves the analysis of degradation from the nanoscale to the mesoscopic scale (Kleibert et al., 2025; B. Li et al., 2024). In addition to resolving inconsistencies in characterization protocols, future PSC research must tackle practical issues like scalable manufacturing, robust encapsulation, and lead-free alternatives. Conflicting reports on ion migration and defect formation have resulted from the absence of standardized operando TEM conditions, such as beam current, temperature, and electrical biasing. To convert nanoscale insights into dependable commercial devices, benchmark protocols must be established through cooperative efforts.

CONCLUSION

This study demonstrates that enhancing the stability and efficiency of PSCs requires not only material optimization but also a basic comprehension of crystal structure dynamics and photovoltaic mechanisms. Energy conversion efficiency is determined by photovoltaic effects, and deep insights into degradation, ion segregation, and microstructure quality are obtained through electron-based characterization. Grain boundaries as recombination centers, halide segregation that lowers Voc and causes hysteresis, and the significance of standardizing characterization techniques were the three primary patterns found in the 15 articles that were examined. In order to balance high efficiency with long-term durability, the research implications highlight the necessity of standardized protocols, operando approaches, and segregation mitigation strategies. By combining the functions of electron diffraction and the photoelectric effect into a single analytical framework, this work adds novelty and lays the groundwork for more focused PSC research.

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