ADVANCEMENTS IN PEROVSKITE SOLAR CELLS: PHYSICS AND MATERIALS PERSPECTIVES

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Submitted: 18/12/2025 Accepted : 30/12/2025

Abstract

Perovskite solar cells (PSCs) have emerged as one of the most transformative photovoltaic technologies of the past decade, demonstrating unprecedented growth in power conversion efficiency from below 4% to over 26% within a short span of research. This rapid progress stems from the unique optoelectronic properties of halide perovskite materials, including tunable bandgaps, long carrier diffusion lengths, and high absorption coefficients. From a physics standpoint, advancements in understanding charge transport, exciton dynamics, and recombination mechanisms have provided critical insights into efficiency improvements. At the same time, materials innovations such as compositional engineering, low-dimensional perovskites, and hybrid organic–inorganic structures have significantly enhanced device stability and environmental resilience. Interface engineering and defect passivation have proven essential in minimizing non-radiative recombination losses and improving long-term operational durability. Furthermore, emerging architectures—such as tandem perovskite–silicon devices, flexible substrates, and scalable deposition techniques—offer promising pathways toward commercial deployment. Despite challenges related to lead toxicity, large-area fabrication, and environmental stability, continuous advances in both physics and materials perspectives suggest a clear trajectory toward industrial-scale applications. This review highlights the synergistic role of fundamental physics and materials engineering in shaping the next generation of PSCs, paving the way for their transition from laboratory prototypes to sustainable, high-performance solar technologies.

Keywords: Perovskite solar cells; photovoltaics; light absorption; charge transport; bandgap tunability; stability; tandem solar cells; defect passivation; interface engineering; materials innovation

Introduction

The global demand for renewable energy has spurred rapid innovation in photovoltaic (PV) technologies, with perovskite solar cells (PSCs) emerging as one of the most promising candidates in the past decade. Since their first demonstration in 2009, PSCs have achieved a meteoric rise in efficiency—from below 4% to over 26%—rivalling crystalline silicon, the dominant material in the solar industry. This remarkable progress is attributed to the exceptional optoelectronic properties of halide perovskites, including strong optical absorption, long carrier diffusion lengths, low exciton binding energies, and facile bandgap tunability. Such attributes have not only accelerated research into the fundamental physics of these materials but also stimulated efforts to engineer more stable, scalable, and environmentally benign perovskite-based devices.

From a physics perspective, PSCs offer unique insights into light–matter interactions. Their broad absorption spectrum and adjustable bandgap enable efficient photon harvesting, while exciton dynamics and charge separation mechanisms differ markedly from traditional semiconductors. Unlike silicon, where excitons are weakly bound, perovskites exhibit hybrid behavior, with low exciton binding energies facilitating free carrier generation under ambient conditions. This interplay between excitonic and free-carrier processes has positioned PSCs as model systems for studying novel photovoltaic physics.

When compared with conventional silicon solar cells, perovskites stand out not only in efficiency potential but also in ease of fabrication. While crystalline silicon requires high-temperature, energy-intensive processes, perovskites can be processed through low-cost solution techniques, offering compatibility with flexible substrates and large-area printing. Thin-film technologies such as CdTe and CIGS (copper indium gallium selenide) have also provided alternatives, but issues of material scarcity, toxicity, and manufacturing costs have limited their scalability. In contrast, perovskites combine performance, tunability, and manufacturing flexibility, although challenges in stability and lead toxicity remain barriers to commercialization.

The rapid progress of PSCs underscores the importance of integrating materials science with device physics. Compositional engineering, through the incorporation of cations (e.g., formamidinium, cesium) and anions (e.g., mixed halides), has significantly improved thermal and moisture stability. Two-dimensional (2D) perovskites, layered structures, and hybrid organic–inorganic frameworks have further enhanced resilience against environmental degradation. At the same time, deeper understanding of charge transport, non-radiative recombination, and interfacial dynamics has informed strategies such as defect passivation, interface engineering, and energy-level alignment. These advancements illustrate how physics-driven insights guide materials innovation and vice versa.

The motivation for continued exploration of PSCs lies not only in achieving higher efficiencies but also in overcoming practical challenges that hinder their large-scale deployment. Scalability to industrial manufacturing, long-term operational stability under outdoor conditions, and mitigation of environmental concerns related to lead remain pressing priorities. Novel device architectures—such as perovskite–silicon tandems, all-perovskite tandems, and flexible modules—highlight the versatility of this technology and its potential to extend beyond traditional rigid panel applications. Moreover, the integration of hot-carrier extraction, photon recycling, and ferroelectric effects may unlock entirely new pathways for efficiency enhancement beyond the Shockley–Queisser limit.

Thus, PSCs represent a unique convergence of physics and materials science, where fundamental understanding of excitonic processes, charge dynamics, and interface phenomena directly informs device engineering and stability strategies. The following sections of this paper discuss in detail the physics of perovskite solar cells, materials innovations driving stability and performance, and the evolution of device architectures that collectively define the roadmap for next-generation PSC technologies.

Section 1: Physics of Perovskite Solar Cells

The performance of perovskite solar cells (PSCs) is underpinned by the unique physical properties of halide perovskite materials. Their favorable optoelectronic characteristics—such as strong absorption, low exciton binding energy, long carrier diffusion lengths, and defect tolerance—enable high power conversion efficiencies (PCEs) and distinguish PSCs from other photovoltaic technologies. A deeper understanding of these physics-related aspects is essential for optimizing device efficiency, stability, and scalability.

1.1 Light Absorption and Bandgap Tunability

One of the most striking features of perovskites is their high absorption coefficient, typically exceeding 10^5 cm^{-1}, which allows films only a few hundred nanometers thick to absorb most of the incident solar spectrum [1]. This property significantly reduces material usage and processing costs compared to crystalline silicon, which requires micrometer-thick wafers.

Equally important is the tunability of the perovskite bandgap through compositional engineering. By adjusting the halide composition (I^-, Br^-, Cl^-) or incorporating different A-site cations (methylammonium, formamidinium, cesium), researchers can tune the bandgap between ~1.2 eV and ~2.3 eV [2]. This flexibility is particularly advantageous for tandem solar cells, where wide-bandgap perovskites (~1.7–1.8 eV) serve as the top cell in perovskite–silicon or all-perovskite tandems. Bandgap engineering also enables spectral matching with the solar spectrum, optimizing photon utilization and reducing thermalization losses.

1.2 Charge Transport Mechanisms

Charge transport in PSCs involves the generation, separation, and extraction of carriers. Unlike traditional semiconductors where excitons (bound electron–hole pairs) dominate, perovskites exhibit low exciton binding energies (<50 meV), which means free carriers are easily generated at room temperature [3]. This leads to efficient charge separation without the need for additional energy input.

Carrier mobility in perovskites is moderate (1–50 $cm^2/V \cdot s$) but sufficient for thin-film architectures

[4]. More importantly, carrier diffusion lengths often exceed 1 µm, far surpassing the typical thickness of perovskite absorber layers (~300–500 nm). This ensures that photogenerated carriers can reach interfaces before recombination, contributing to high open-circuit voltages and fill factors.

1.3 Recombination Pathways and Defect States

Recombination processes in PSCs can be classified as radiative, Shockley–Read–Hall (trap-assisted), or Auger recombination. Radiative recombination, which occurs when electrons recombine with holes emitting photons, is an unavoidable but relatively benign process [5]. Trap-assisted recombination, however, is a major efficiency loss pathway in PSCs. Defects such as halide vacancies, interstitials, and grain-boundary states act as recombination centers, reducing carrier lifetimes and device performance [6].

Remarkably, halide perovskites exhibit a high level of “defect tolerance,” meaning many intrinsic defects have shallow energy levels and thus do not severely affect carrier transport. This contrasts with conventional semiconductors like GaAs, where even small defect densities can drastically reduce performance [7]. Nonetheless, minimizing deep-level defects through strategies like compositional engineering, additive incorporation, and passivation remains crucial for further efficiency gains.

1.4 Role of Interfaces and Energy-Level Alignment

In PSCs, interfaces between the perovskite absorber and charge transport layers (CTLs) play a pivotal role in determining efficiency and stability. Mismatched energy levels between the absorber and transport layers can create energy barriers, hindering carrier extraction and promoting recombination [8].

For instance, an ideal electron transport layer (ETL) should align well with the conduction band of the perovskite, while the hole transport layer (HTL) should align with the valence band. Materials such as TiO_2, SnO_2, and ZnO have been widely used as ETLs, while spiro-OMeTAD and PTAA serve as common HTLs [9]. Recent research highlights that interface engineering—through self-assembled monolayers, 2D perovskite passivation layers, or molecular interlayers—significantly reduces recombination losses and enhances stability [10].

Moreover, interfacial defects, including dangling bonds and trap states, accelerate non-radiative recombination. Passivation strategies that involve fullerene derivatives, alkali-metal halides, or organic ammonium salts have been shown to mitigate these issues, yielding higher open-circuit voltages and longer device lifetimes.

1.5 Novel Physics Concepts in Perovskite Solar Cells

Beyond conventional mechanisms, PSCs exhibit novel physical phenomena that offer pathways to surpass the efficiency limits of traditional photovoltaics.

- **Hot-Carrier Extraction:** Halide perovskites demonstrate slow hot-carrier cooling compared to silicon, meaning that photogenerated carriers retain excess energy for longer periods before thermalizing to the band edges [11]. Harnessing these “hot carriers” could theoretically allow efficiencies beyond the Shockley–Queisser limit. Although practical hot-carrier solar cells remain unrealized, experimental studies show that energy-selective contacts may exploit this effect in perovskite absorbers.
- **Ferroelectric Effects:** Some perovskite compositions exhibit ferroelectric-like polarization, which may assist in separating electron–hole pairs and reducing recombination [12]. While the exact contribution of ferroelectricity to device operation is debated, local polarization domains and ion migration phenomena are thought to influence hysteresis behavior in current–voltage curves.
- **Photon Recycling:** Perovskites exhibit strong photoluminescence and high radiative efficiencies, enabling photon recycling, where re-emitted photons are reabsorbed and contribute to photocurrent [13]. This effect can enhance open-circuit voltage and boost device efficiency if optimized through optical design and encapsulation strategies.

Materials Perspectives

The rapid advancement of perovskite solar cells (PSCs) has been driven not only by their unique physics but also by continuous innovations in materials design. Material composition, dimensionality, and chemical engineering directly determine the optoelectronic performance, stability, and scalability of PSCs. Key directions include the development of 3D vs 2D perovskite structures, compositional engineering for improved stability and reduced toxicity, the use of additives and dopants to optimize defect passivation, and encapsulation strategies to mitigate degradation.

2.1 Development of 3D vs 2D Perovskite Structures

The prototypical perovskite used in photovoltaics follows the 3D ABX_3 structure, where A is a monovalent cation (methylammonium, formamidinium, or cesium), B is a metal cation (commonly Pb^{2+} or Sn^{2+}), and X is a halide anion (I^-, Br^-, Cl^-). These 3D structures offer superior charge transport and light absorption properties, making them the workhorse of high-efficiency PSCs [14]. However, their inherent instability against moisture, oxygen, and thermal stress has limited long-term operational lifetimes.

To address this, 2D perovskites—composed of alternating inorganic layers and bulky organic spacer cations—have been explored. These Ruddlesden–Popper structures exhibit enhanced environmental stability due to hydrophobic organic layers that protect the inorganic framework [15]. Although 2D perovskites generally show lower carrier mobility and reduced efficiency compared to 3D analogues, hybrid 2D/3D perovskite heterostructures combine the efficiency of 3D perovskites with the robustness of 2D materials. This has become a promising approach for balancing stability and performance in practical devices.

2.2 Compositional Engineering: Organic–Inorganic and Lead-Free Alternatives

Early PSCs were dominated by methylammonium lead iodide ($MAPbI_3$), but its poor thermal stability and sensitivity to moisture spurred the development of alternative compositions. Formamidinium-based ($FAPbI_3$) and cesium-based perovskites have demonstrated improved structural stability and higher thermal tolerance [16]. Multi-cation systems, such as triple-cation perovskites (FA–MA–Cs), further enhance both stability and reproducibility by suppressing undesirable phase transitions.

On the anion side, mixed-halide perovskites (I/Br or I/Cl combinations) allow bandgap tuning while reducing halide migration. However, light-induced halide segregation remains a challenge, causing long-term instability in mixed-halide devices [17].

Given concerns about lead toxicity, alternative B-site cations such as Sn^{2+}, Ge^{2+}, and Bi^{3+} have been investigated. Tin-based perovskites (e.g., $MASnI_3$) offer bandgaps similar to Pb-based analogues but suffer from rapid oxidation of Sn^{2+} to Sn^{4+}, leading to poor stability and low efficiency [18]. Bi- and Sb-based double perovskites ($A_2B'B''X_6$) are lead-free alternatives with better stability and non-toxicity, though they often exhibit indirect bandgaps and limited efficiencies. While lead remains the benchmark for high efficiency, research into lead-free alternatives continues to expand, especially for environmentally sustainable applications.

2.3 Additives and Dopants for Stability and Performance

The incorporation of small amounts of additives and dopants has proven to be an effective way to improve perovskite film quality, defect passivation, and operational stability.

- **Halide Additives:** Excess halides, such as iodide salts, can passivate halide vacancies and suppress non-radiative recombination [19].
- **Alkali-Metal Dopants:** Cesium, rubidium, and potassium ions improve crystallinity, reduce defect density, and stabilize the perovskite lattice.
- **Molecular Additives:** Compounds such as fullerene derivatives, thiocyanates, and Lewis bases have been introduced to passivate trap states and enhance film uniformity [20].
- **Redox Additives:** In tin-based perovskites, reducing agents such as SnF_2 help suppress Sn^{2+} oxidation, improving both device performance and stability.

These strategies exemplify how minor compositional modifications at the nanoscale can yield major improvements in efficiency and durability.

2.4 Encapsulation and Degradation Pathways

A critical challenge for PSC commercialization lies in their vulnerability to moisture, oxygen, UV radiation, and thermal stress. Perovskite materials degrade through several pathways, including ion migration, phase segregation, and decomposition into PbI_2 under humid conditions [21]. Encapsulation strategies are therefore essential to prolong device lifetimes.

Polymeric encapsulants, glass covers, and atomic-layer-deposited (ALD) oxide barriers are commonly employed to protect perovskite layers from the environment. Recent studies also highlight the role of interface engineering in mitigating degradation by suppressing ion migration and stabilizing contact layers [22]. Additionally, 2D perovskite capping layers act as intrinsic encapsulants, enhancing hydrophobicity and chemical robustness.

Despite these advancements, achieving operational stability beyond 20 years—comparable to silicon modules—remains an unsolved challenge. Encapsulation must therefore be combined with intrinsic material stability improvements to enable large-scale commercialization.

Device Architectures and Engineering

Device architecture is a crucial determinant of PSC performance, as it governs light absorption, charge transport, recombination, and stability. Over the past decade, diverse architectures have been developed, ranging from conventional planar and mesoporous structures to advanced tandem devices, flexible modules, and interface-engineered systems.

3.1 Planar vs Mesoporous Structures

The two most common architectures are planar heterojunctions and mesoporous scaffolds.

- **Planar Structures:** These consist of a flat perovskite absorber sandwiched between transport layers. They offer simplicity in fabrication and compatibility with low-temperature processing [23]. Planar devices are particularly attractive for flexible and tandem applications.
- **Mesoporous Structures:** These incorporate a mesoporous oxide scaffold (e.g., TiO_2) that facilitates charge separation and enhances mechanical stability. Early PSCs used mesoporous TiO_2, but its high-temperature sintering and UV instability have driven a shift toward planar configurations [24].

Planar devices have largely overtaken mesoporous ones due to their scalability and reproducibility, although hybrid architectures combining aspects of both remain under exploration.

3.2 Tandem Perovskite–Silicon Devices

Perovskite–silicon tandems have emerged as one of the most promising routes to surpass the single-junction efficiency limit (~33%). By stacking a wide-bandgap perovskite top cell (~1.7 eV) on a silicon bottom cell (~1.1 eV), tandem devices can harvest complementary portions of the solar spectrum, achieving record efficiencies above 33% [25].

Two main architectures exist:

- **Two-Terminal (Monolithic):** Both cells are connected in series, requiring careful current matching between subcells.
- **Four-Terminal (Mechanically Stacked):** Each subcell operates independently, simplifying fabrication but adding cost and complexity.

Tandems demonstrate how perovskites can complement, rather than replace, established silicon technologies, accelerating their path toward commercialization.

3.3 Flexible and Printable PSCs

One of the unique advantages of PSCs is their compatibility with solution processing and low-temperature fabrication, enabling flexible, lightweight, and printable solar cells. Perovskite films can be deposited by techniques such as spin-coating, blade-coating, slot-die coating, and inkjet printing [26]. This allows integration into wearable electronics, building-integrated photovoltaics (BIPV), and portable devices.

Flexible PSCs fabricated on plastic substrates have achieved efficiencies exceeding 20%, highlighting their potential for next-generation energy applications. However, mechanical durability and encapsulation under repeated bending remain challenges that require further engineering.

3.4 Interface Passivation Strategies

Interfaces remain one of the most critical bottlenecks in PSCs, as they dictate charge extraction efficiency and stability. Imperfect interfaces between the perovskite absorber and transport layers introduce trap states, which accelerate non-radiative recombination. Passivation strategies are therefore essential for achieving high efficiency.

Common approaches include:

- **Organic Passivation:** Using alkylammonium salts or polymers to passivate grain boundaries.
- **Inorganic Passivation:** Employing metal oxides (e.g., Al_2O_3, MgO) to create barrier layers that suppress ion migration.
- **2D Perovskite Passivation:** Depositing ultrathin 2D layers on top of 3D perovskites to form stable heterojunctions [27].

These strategies not only improve efficiency but also enhance long-term operational stability, making interface passivation a cornerstone of next-generation PSC design.

Discussion & Challenges

Despite remarkable efficiency gains, perovskite solar cells face significant challenges that hinder their large-scale adoption. The most pressing issue is stability. Perovskite materials degrade under moisture, oxygen, ultraviolet light, and thermal stress, leading to rapid performance loss. Ion migration and phase segregation further accelerate this degradation. While compositional engineering and encapsulation strategies have improved operational lifetimes, achieving stability comparable to silicon modules over 20–25 years remains unresolved.

Scalability is another major concern. Most record-breaking devices are fabricated on small areas under laboratory conditions using spin-coating, a technique unsuitable for industrial-scale production. Transitioning to scalable methods such as blade coating, slot-die coating, or vapor deposition introduces challenges in achieving film uniformity, defect control, and reproducibility across large modules. Moreover, integration with existing photovoltaic manufacturing infrastructure requires compatibility with established processing techniques and supply chains.

Toxicity, particularly due to lead content in the most efficient perovskites, poses both environmental and regulatory concerns. Although the absolute amount of lead per module is small, risks associated with lead leakage during production, use, or disposal must be addressed. Lead-free alternatives, such as tin- or bismuth-based perovskites, remain under investigation but have yet to match the efficiency and stability of lead-based counterparts.

Industrialization and commercialization barriers stem from the combination of these issues. Investors and manufacturers are cautious about committing to perovskite technology until long-term reliability, large-area scalability, and regulatory compliance are demonstrated. The field must therefore balance scientific innovation with practical engineering solutions.

Looking ahead, the future of perovskite research lies in the convergence of physics insights and materials innovations. New approaches such as tandem architectures, flexible devices, and interface passivation offer promising directions. At the same time, deeper understanding of degradation mechanisms and the development of robust encapsulation strategies will be critical for achieving commercial viability.

Conclusion

Perovskite solar cells have rapidly transformed the photovoltaic landscape, achieving efficiencies that rival silicon within just over a decade of research. This success is grounded in their unique physics, including strong optical absorption, low exciton binding energies, long carrier diffusion lengths, and defect tolerance. These properties enable efficient light harvesting and charge transport, while novel concepts such as photon recycling, hot-carrier effects, and ferroelectric polarization open pathways for surpassing classical efficiency limits.

Equally transformative have been the advances in materials design. Compositional engineering has yielded perovskites with enhanced stability and tunable bandgaps, while 2D and mixed-dimensional structures combine efficiency with resilience. Additives and dopants have improved crystallinity, defect passivation, and device reproducibility, whereas encapsulation and interface engineering have extended operational lifetimes. These materials innovations directly complement physics-driven insights, together shaping the trajectory of perovskite solar research.

Device architectures have evolved in parallel, from mesoporous and planar single-junction devices to advanced tandem structures that surpass the single-junction efficiency limit. Flexible and printable PSCs further highlight the versatility of this technology, enabling integration into diverse applications beyond traditional solar panels.

The challenges of stability, scalability, and toxicity remain formidable, yet continuous progress suggests that solutions are within reach. The roadmap to commercialization will depend on integrating intrinsic material stability with scalable processing techniques, environmentally responsible designs, and industry-compatible encapsulation strategies.

In summary, the synergy between physics and materials perspectives has propelled perovskite solar cells to the forefront of next-generation photovoltaics. With sustained innovation, PSCs hold the potential to become a commercially viable, sustainable, and high-performance alternative to conventional solar technologies, shaping the future of renewable energy.

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