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Perovskite Materials: Properties, Advancements, and Emerging Applications

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Abstract— Perovskite materials have emerged as a highly promising class of functional materials for next-generation energy and optoelectronic applications due to their unique crystal structure, tunable bandgaps, strong light absorption, and low-temperature process ability. Over the past decade, perovskite solar cells have demonstrated unprecedented improvements in power conversion efficiency, rivaling and surpassing conventional photovoltaic technologies, while also enabling tandem architectures with silicon. Beyond photovoltaics, perovskites have shown exceptional potential in light-emitting diodes, photodetectors, lasers, energy storage integration, and emerging applications such as building-integrated photovoltaics, agrivoltaics, space systems, and wearable electronics. Despite these advances, challenges related to long-term operational stability, environmental concerns associated with lead content, and large-scale manufacturing remain key barriers to commercialization. This review provides a comprehensive overview of the crystal structure, fundamental properties, device physics, and recent technological progress of perovskite-based systems, while critically examining current limitations and future research directions. Continued advances in materials engineering, scalable fabrication, and data-driven optimization, coupled with strong interdisciplinary collaboration, are expected to accelerate the transition of perovskite technologies from laboratory research to commercial deployment.

Keywords—Perovskite materials, solar cells, optoelectronics, tandem photovoltaics, energy applications

I. INTRODUCTION

The global transition toward clean and sustainable energy systems has intensified scientific and technological efforts to develop advanced materials capable of delivering high efficiency, long-term stability, and cost-effective manufacturing¹. In this context, photovoltaic technologies play a central role in mitigating climate change and reducing dependence on fossil fuels. Among emerging photovoltaic materials, perovskite compounds have gained extraordinary attention owing to their remarkable optoelectronic properties, compositional versatility, and solution-processable fabrication routes, positioning them as strong contenders for next-generation solar energy conversion technologies².

Perovskite materials are defined by the general crystal structure ABX_3 , where the A-site cation is typically an organic or inorganic monovalent ion (e.g., methyl ammonium, form amidinium, or cesium), the B-site cation is a divalent metal ion (commonly lead or tin), and X represents a halide or oxide anion³. This flexible lattice architecture enables extensive chemical substitution, allowing precise tuning of structural, optical, and electronic properties¹. As a result, perovskites exhibit high absorption coefficients, long charge-carrier diffusion lengths, low exciton binding energies, and pronounced defect tolerance—characteristics that are highly advantageous for efficient photovoltaic operation⁴.

The application of hybrid organic–inorganic halide perovskites in solar cells was first reported in 2009, when Kojima et al. demonstrated power conversion efficiencies of approximately 3% using methylammonium lead halide sensitizers³. Following this seminal discovery, perovskite solar cell (PSC) technology has evolved at an unprecedented pace, driven by rapid advances in material composition, crystallization control, interfacial passivation, and device engineering⁵. These developments have enabled certified power conversion efficiencies of single-junction PSCs to exceed 25%, approaching those of commercial crystalline silicon solar cells⁵.

More recently, tandem solar cell architectures that combine perovskite absorbers with crystalline silicon have emerged as a promising strategy to overcome the Shockley–Queisser efficiency limit of single-junction devices¹. Owing to their tunable bandgaps, perovskites are ideally suited as wide-bandgap top absorbers in perovskite–silicon tandem configurations⁶. Consequently, monolithic tandem devices have achieved certified efficiencies exceeding 30%, underscoring the synergistic potential of integrating perovskite materials with mature silicon technologies⁶.

Despite these remarkable advances, several critical challenges hinder the large-scale commercialization of perovskite photovoltaics.

In particular, intrinsic material instability under exposure to moisture, oxygen, heat, and prolonged illumination remains a major concern, along with ion migration, interfacial degradation, and long-term operational reliability^{4,7}. Furthermore, environmental concerns associated with lead toxicity and the scalability of fabrication processes necessitate continued innovation in material design, encapsulation strategies, and sustainable manufacturing approaches⁸.

Nonetheless, ongoing research focused on compositional engineering, additive incorporation, interface optimization, and advanced encapsulation has yielded substantial improvements in device stability and reproducibility^{5,6}. These developments, combined with the low-temperature, solution-processable nature of perovskite materials, highlight their strong potential for enabling high-efficiency, low-cost photovoltaic technologies suitable for widespread deployment.

II. CRYSTAL STRUCTURE AND FUNDAMENTAL PROPERTIES

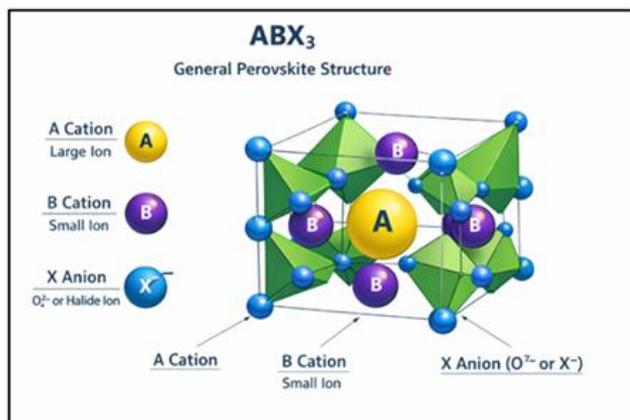


Figure 1. General crystal structure of perovskite (ABX₃). The A-site cation is located at the corners of the unit cell, the B-site cation is at the center, and the X-site anions surround the B-site to form BX₆ octahedra.

Perovskites are a broad class of materials defined by the characteristic crystal structure with the general chemical formula ABX₃, where A and B are cations of differing ionic radii and X is an anion, typically oxygen or a halide^{3,9}. In the ideal perovskite structure, the larger A-site cation occupies a cuboctahedral cavity formed by corner-sharing BX₆ octahedra, while the smaller B-site cation resides at the center of the octahedron. This three-dimensional framework provides exceptional structural flexibility, enabling a wide range of chemical substitutions without destabilizing the lattice¹⁰.

The stability and symmetry of the perovskite lattice are commonly assessed using the Goldschmidt tolerance factor (*t*), which relates the ionic radii of the constituent ions. For stable perovskite formation, the tolerance factor typically lies between 0.8 and 1.0, with deviations resulting in octahedral tilting, lattice distortion, or phase transitions to lower-symmetry structures such as tetragonal or orthorhombic phases^{10,11}. These structural distortions significantly influence electronic band structure, carrier mobility, and optical absorption, thereby directly affecting device performance.

Hybrid organic–inorganic halide perovskites, in which the A-site is occupied by organic cations such as methylammonium (CH₃NH₃⁺) or formamidinium (HC(NH₂)₂⁺), exhibit dynamic lattice behavior arising from the rotational motion of the organic moieties⁹. This dynamic disorder contributes to strong dielectric screening and reduced Coulombic interactions between charge carriers, leading to low exciton binding energies and efficient charge separation at room temperature⁴. In contrast, all-inorganic perovskites, such as cesium lead halides, display enhanced thermal stability but often require compositional engineering to achieve phase stability under ambient conditions¹².

From an electronic perspective, perovskites exhibit direct bandgaps that are highly tunable through compositional modification of the A-, B-, and X-site ions¹³. Substitution of halide ions enables precise control over the bandgap across the visible spectrum, making perovskites particularly attractive for optoelectronic applications, including photovoltaics, light-emitting diodes, and photodetectors. Furthermore, the electronic band structure of metal halide perovskites is characterized by antibonding valence band maxima and conduction band minima, which confer exceptional defect tolerance by minimizing the formation of deep trap states within the bandgap¹⁴.

Optically, perovskites possess high absorption coefficients on the order of 10⁴–10⁵ cm⁻¹, allowing efficient light harvesting with absorber layers only a few hundred nanometers thick¹. Combined with long charge-carrier diffusion lengths and lifetimes—often exceeding micrometer scales—these properties facilitate efficient charge collection even in polycrystalline thin films⁴. Additionally, relatively low effective masses for electrons and holes contribute to high carrier mobilities, further enhancing photovoltaic performance.

The ionic nature of the perovskite lattice also introduces unique phenomena such as ion migration under electric fields or illumination, which can influence device hysteresis and long-term stability⁷.

While ion migration poses challenges for device reliability, it also offers opportunities for novel functionalities, including defect self-healing and adaptive optoelectronic behavior. Consequently, understanding the interplay between crystal structure, electronic properties, and ionic dynamics remains central to advancing perovskite-based technologies.

III. PEROVSKITE SOLAR CELLS

A. Working Principle

Perovskite solar cells (PSCs) operate on the principle of photovoltaic conversion, wherein incident photons are absorbed by the perovskite absorber layer, leading to the generation of free charge carriers in the form of electron–hole pairs. Owing to the low exciton binding energy of metal-halide perovskites, these photogenerated carriers readily dissociate at room temperature. The electrons and holes are selectively transported through electron transport layers (ETLs) and hole transport layers (HTLs), respectively, before being collected at the corresponding electrodes to produce electrical power^{2,4}.

A defining advantage of PSCs lies in their relatively simple device architecture, which can be realized in mesoporous, planar heterojunction, or inverted configurations. Moreover, the solution-processable nature of perovskite materials enables low-temperature fabrication, reduced energy consumption, and compatibility with flexible substrates—features that clearly distinguish PSCs from conventional crystalline silicon photovoltaics¹.

B. Efficiency Advancements

The rapid rise in power conversion efficiency of PSCs is primarily attributed to advances in compositional engineering, defect passivation, and interface optimization. In particular, mixed-cation (e.g., formamidinium–methylammonium–cesium) and mixed-halide perovskite formulations have significantly enhanced phase stability, suppressed non-radiative recombination, and improved charge-carrier lifetimes¹⁵. Simultaneously, passivation strategies employing small molecules, polymers, and ionic additives have effectively reduced defect densities at grain boundaries and interfaces, resulting in higher open-circuit voltages and fill factors^{5,14}.

Beyond single-junction devices, tandem solar cell architectures have emerged as a transformative strategy for further efficiency enhancement.

Perovskite–silicon tandem cells, in which a wide-bandgap perovskite top cell is integrated with a silicon bottom cell, enable more efficient utilization of the solar spectrum and overcome the Shockley–Queisser efficiency limit of single-junction silicon devices⁶. Such tandem configurations have now achieved efficiencies exceeding 30%, underscoring the exceptional potential of perovskite materials for next-generation photovoltaic technologies.

C. Stability and Scalability Challenges

Despite their impressive efficiency gains, the long-term stability and large-scale manufacturability of PSCs remain critical challenges. Metal-halide perovskites are inherently sensitive to environmental stressors such as moisture, oxygen, heat, and prolonged illumination, which can induce phase segregation, ion migration, and irreversible material degradation⁷. Thermal instability and operational degradation under real-world conditions continue to limit device lifetimes compared to established photovoltaic technologies.

In addition, environmental and regulatory concerns related to the presence of lead in most high-performance perovskite formulations pose significant barriers to commercialization⁸. Although the absolute lead content in PSCs is relatively low, potential leakage during device failure necessitates robust mitigation strategies. Current research efforts are therefore focused on advanced encapsulation techniques, development of lead-free or reduced-lead perovskite compositions, and scalable deposition methods such as blade coating, slot-die coating, and vapor-based processing to enable industrial-scale production^{5,16}.

IV. OPTOELECTRONIC APPLICATIONS BEYOND PHOTOVOLTAICS

Beyond their prominent role in solar energy conversion, metal-halide perovskites have emerged as versatile materials for a wide range of optoelectronic applications. Their exceptional photoluminescence quantum yields, tunable bandgaps, narrow emission linewidths, and solution-processable fabrication make them particularly attractive for light-emitting devices, photodetectors, and coherent light sources.

A. Light-Emitting Diodes

Perovskite light-emitting diodes (PeLEDs) have witnessed rapid performance improvements over the past decade, driven by advances in material composition, dimensional engineering, and defect passivation.

The direct bandgap nature of metal-halide perovskites, combined with high radiative recombination rates and low defect densities, enables efficient electroluminescence with high color purity⁴. By tuning the halide composition and crystal dimensionality, emission wavelengths can be precisely controlled across the visible spectrum and into the near-infrared region¹⁷.

Recent developments in quasi-two-dimensional and nanocrystalline perovskite structures have significantly enhanced exciton confinement and suppressed non-radiative losses, leading to external quantum efficiencies (EQEs) exceeding 20% in green and red PeLEDs¹⁸. These performance metrics, combined with low-temperature, solution-based processing and compatibility with flexible substrates, position perovskite emitters as promising candidates for next-generation solid-state lighting and high-resolution display technologies.

B. Photodetectors and Lasers

Perovskite-based photodetectors have attracted considerable attention due to their strong optical absorption, long carrier diffusion lengths, and low dark current densities. These properties enable high responsivity, fast temporal response, and broad spectral sensitivity spanning the ultraviolet to near-infrared regions¹⁹. Additionally, the facile tunability of perovskite bandgaps allows wavelength-selective photodetection without the need for complex heterostructures, making them well suited for applications in imaging, environmental monitoring, and optical sensing.

Perovskites have also demonstrated outstanding potential as gain media for laser applications. Their high optical gain coefficients, low exciton binding energies, and efficient radiative recombination facilitate low lasing thresholds under optical pumping²⁰. Moreover, perovskite micro- and nanostructures—including nanowires, microplates, and distributed feedback cavities—enable wavelength-tunable lasing across the visible spectrum. These attributes make perovskite lasers attractive for integrated photonics, optical communication systems, and on-chip coherent light sources.

Despite these promising advances, challenges related to operational stability, ion migration, and thermal management remain significant obstacles for the long-term deployment of perovskite-based optoelectronic devices. Continued research into compositional engineering, encapsulation strategies, and device architecture optimization is therefore essential to fully exploit the optoelectronic potential of perovskite materials beyond photovoltaics.

C. Energy Storage and Hybrid Systems

In addition to their prominent roles in photovoltaics and optoelectronics, perovskite materials are increasingly being investigated for applications in energy storage and integrated hybrid energy systems. The rapid growth of solar power generation has highlighted the critical need for efficient energy storage solutions to address the inherent intermittency and temporal mismatch between energy generation and consumption. In this context, hybrid systems that integrate perovskite-based solar cells with electrochemical energy storage devices, such as lithium-ion and solid-state batteries, have emerged as a promising strategy for achieving stable and continuous power supply.

The suitability of perovskite materials for hybrid energy systems stems from their favorable electronic and ionic transport properties, as well as their compatibility with low-temperature, solution-based fabrication processes. Metal-halide perovskites exhibit mixed ionic–electronic conductivity, which can facilitate efficient charge transfer and interfacial coupling when integrated with battery electrodes or solid electrolytes^{21,22}. This unique transport behavior has stimulated interest in perovskite materials not only as light absorbers but also as functional components in energy storage architectures.

Recent studies have demonstrated the feasibility of perovskite–battery integration through direct coupling of perovskite solar cells with lithium-ion batteries, enabling on-site energy harvesting and storage within compact device configurations²³. Such integrated solar–battery platforms reduce system complexity and energy losses associated with external power management components. Furthermore, the tunable bandgap and high output voltage of perovskite solar cells are particularly advantageous for efficiently charging high-voltage battery systems, including emerging solid-state batteries.

Beyond direct integration, perovskite materials have also been explored as electrode additives, interfacial layers, and ion-conducting components in next-generation batteries. Their soft lattice structure and defect tolerance can accommodate ion migration, which, when properly controlled, may enhance interfacial stability and electrochemical performance²⁴. However, challenges related to chemical stability, ion migration-induced degradation, and long-term operational reliability must be carefully addressed before large-scale deployment of perovskite-based hybrid systems becomes feasible.

Overall, the integration of perovskite materials into energy storage and hybrid energy platforms represents a rapidly evolving research frontier.

Continued advances in materials engineering, interface design, and device integration strategies are expected to play a pivotal role in enabling efficient, durable, and scalable solutions for renewable energy generation and storage.

V. EMERGING APPLICATIONS

Beyond conventional photovoltaic deployment, the unique physical, optical, and mechanical properties of perovskite materials have enabled a broad spectrum of emerging applications. Their tuneable bandgaps, high absorption coefficients, low-temperature processability, and mechanical flexibility offer advantages that are difficult to achieve with established photovoltaic technologies, thereby expanding the functional scope of perovskite-based devices.

A. Building-Integrated Photovoltaics

Building-integrated photovoltaics (BIPV) represent a rapidly growing application area in which energy generation is seamlessly incorporated into architectural elements such as windows, façades, and rooftops. Perovskite materials are particularly well suited for BIPV due to their lightweight nature, semi-transparency, and tunable optical properties. By adjusting composition and thickness, perovskite absorbers can selectively transmit visible light while harvesting ultraviolet and near-infrared radiation, enabling electricity generation without significantly compromising indoor illumination or visual aesthetics^{12,25}.

Furthermore, the compatibility of perovskites with solution-based and low-temperature fabrication allows deposition on large-area glass and flexible substrates, which is advantageous for retrofitting existing buildings and reducing overall installation costs. Semi-transparent perovskite modules have demonstrated promising power conversion efficiencies while maintaining high average visible transmittance, highlighting their potential as multifunctional building components that contribute simultaneously to energy efficiency and architectural design²⁶.

B. Space and Wearable Electronics

Perovskite solar cells have also attracted significant interest for space and aerospace applications, where high power-to-weight ratios and radiation tolerance are critical performance metrics.

The high specific power of perovskite photovoltaics enables substantial reductions in payload mass compared to conventional space-grade solar panels, offering clear advantages for satellites and deep-space missions²⁷. Experimental studies have further indicated that perovskite materials exhibit notable resistance to proton and electron irradiation, making them promising candidates for operation in harsh space environments.

In parallel, the mechanical flexibility and low-temperature processability of perovskite devices enable their integration into wearable and portable electronics. Flexible perovskite solar cells fabricated on polymer substrates can conform to curved surfaces and maintain performance under mechanical deformation, supporting applications in self-powered sensors, smart textiles, and portable electronic devices²⁸. These characteristics position perovskite materials as key enablers of next-generation, lightweight energy-harvesting technologies.

C. Agrivoltaics and Environmental Monitoring

Agrivoltaic systems aim to combine agricultural productivity with renewable energy generation by deploying photovoltaic modules that allow partial light transmission to underlying crops. Semi-transparent perovskite solar cells are particularly attractive for such systems due to their wavelength-selective absorption, which can be engineered to optimize both photosynthetically active radiation for plant growth and electrical power output²⁹. This dual functionality offers a sustainable pathway to maximize land-use efficiency while addressing growing energy and food demands.

In addition to energy harvesting, perovskite materials have demonstrated considerable potential in environmental sensing and monitoring applications. Their high sensitivity to light, gases, and chemical species, combined with fast response times, enables the development of perovskite-based photodetectors and sensors for monitoring air quality, radiation levels, and environmental pollutants²⁴. As research continues to improve device stability and selectivity, perovskite-based sensors are expected to play an increasingly important role in environmental monitoring and smart infrastructure systems.

VI. FUTURE PROSPECTS

The continued advancement and eventual commercialization of perovskite-based technologies critically depend on addressing persistent challenges related to long-term operational stability, environmental safety, and large-scale manufacturability.

Although remarkable progress has been achieved in improving device efficiency and short-term stability, perovskite materials remain vulnerable to degradation induced by moisture, heat, oxygen, and prolonged illumination. Future research must therefore focus on intrinsically stable perovskite compositions, advanced encapsulation strategies, and robust interface engineering to ensure device lifetimes compatible with commercial photovoltaic standards^{5,7}.

Toxicity concerns, particularly those associated with lead-containing perovskites, represent another major obstacle to widespread adoption. While the absolute lead content in perovskite devices is relatively low, regulatory and environmental considerations necessitate the development of effective mitigation strategies. These include lead sequestration layers, recycling protocols, and the exploration of lead-free or reduced-lead alternatives based on tin, germanium, or double-perovskite structures^{8,16}. Balancing environmental safety with high device performance remains a key challenge for future materials design.

Scalability and manufacturing reproducibility are equally critical for commercial deployment. Transitioning from laboratory-scale spin coating to industrially viable fabrication techniques—such as slot-die coating, blade coating, inkjet printing, and vapor-phase deposition—requires precise control over film uniformity, defect density, and interfacial quality across large areas³⁰. Continued efforts in process optimization and standardization will be essential to bridge the gap between small-area devices and commercially relevant module-scale production.

Looking ahead, the integration of artificial intelligence (AI) and machine learning (ML) is expected to play a transformative role in accelerating perovskite research and development. Data-driven approaches enable rapid screening of compositional spaces, prediction of material stability, and optimization of device architectures, significantly reducing experimental trial-and-error^{31,32}. The synergistic combination of high-throughput experimentation and ML-assisted modeling is likely to shorten development cycles and facilitate the discovery of robust, high-performance perovskite systems.

Finally, strong and sustained collaboration among academia, industry, and policymakers will be indispensable for translating laboratory breakthroughs into commercially viable technologies. Academic research provides fundamental insights and innovation, while industrial partnerships enable scale-up, reliability testing, and market integration.

Concurrently, supportive regulatory frameworks and standardized testing protocols will be necessary to ensure environmental safety, consumer confidence, and long-term deployment. Through coordinated interdisciplinary efforts, perovskite technologies are poised to play a pivotal role in the future global energy landscape.

VII. CONCLUSION

In summary, perovskite materials represent a highly versatile and rapidly advancing class of functional materials with transformative potential across photovoltaics, optoelectronics, energy storage, and emerging hybrid applications. Their distinctive crystal structure, tunable optoelectronic properties, and low-temperature processability have enabled unprecedented gains in power conversion efficiency, device functionality, and application diversity, ranging from tandem solar cells and light-emitting diodes to building-integrated photovoltaics and integrated energy systems. While critical challenges related to long-term stability, environmental safety, and scalable manufacturing remain, sustained progress in compositional engineering, interface design, encapsulation strategies, and data-driven materials discovery continues to push perovskite technologies closer to commercial viability. With coordinated efforts spanning fundamental research, industrial scale-up, and supportive policy frameworks, perovskite-based technologies are well positioned to play a central role in enabling efficient, sustainable, and multifunctional energy solutions for the future.

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