

Inorganic Perovskite Materials for Solar Cells and Optoelectronics: Stability, Efficiency, and Future Prospects — A Review

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I. INTRODUCTION

The global imperative to transition from fossil fuel-based energy systems toward renewable alternatives has catalyzed an unprecedented surge of research into advanced photovoltaic technologies. Among the most disruptive developments of the past decade has been the meteoric rise of metal halide perovskite solar cells, which have progressed from a power conversion efficiency (PCE) of 3.8% in 2009 to certified efficiencies exceeding 26% for single-junction devices as of 2025 (NREL, 2025). This trajectory of improvement, unparalleled in the history of photovoltaics, reflects both the exceptional intrinsic optoelectronic properties of perovskite semiconductors and the intensive global research

effort directed toward their optimization (Stranks & Snaith, 2015).

Metal halide perovskites adopt the general formula ABX_3 , where A is a monovalent cation (e.g., methylammonium $[MA^+]$, formamidinium $[FA^+]$, or Cs^+), B is a divalent metal cation (typically Pb^{2+} or Sn^{2+}), and X is an halide anion (I^- , Br^- , or Cl^-). The field initially achieved its most celebrated milestones using hybrid organic–inorganic perovskites (HOIPs), particularly $MAPbI_3$. However, the inherent sensitivity of organic cations to moisture, oxygen, heat, and illumination imposes severe constraints on the long-term operational stability of HOIP-based devices a critical requirement for commercial viability (Chen et al., 2015). The limitations associated with the stability have motivated intensive investigation of all-

inorganic perovskites, in which the volatile organic A-site cation is replaced by the inorganic caesium ion (Cs^+).

Inorganic perovskites, particularly CsPbX_3 compositions, offer several compelling advantages such as substantially enhanced thermal stability (capable of withstanding temperatures exceeding 300°C without structural decomposition), resistance to phase segregation under illumination, compatibility with high-temperature annealing processes used in industrial device fabrication, and the ability to form both bulk thin films and quantum confined nanostructures with tunable emission properties. These characteristics, combined with bandgaps that can be continuously tuned from approximately 1.73 eV (CsPbI_3) to 2.36 eV (CsPbBr_3) through halide composition adjustment, render inorganic perovskites particularly attractive for applications ranging from single-junction photovoltaics to tandem cells, LEDs, photodetectors, lasers, and X-ray imaging sensors (Eperon et al., 2015).

Nevertheless, the commercialization of inorganic perovskite technologies confronts substantial challenges. The thermodynamic instability of the photoactive black-phase CsPbI_3 (alpha-phase) at room temperature which reverts to a non-perovskite yellow delta-phase under ambient conditions represents perhaps the most fundamental obstacle for iodide-rich compositions. Furthermore, the toxicity associated with lead-based formulations raises serious environmental and regulatory concerns, driving parallel efforts toward lead-free alternatives including CsSnI_3 , $\text{Cs}_2\text{AgBiBr}_6$ (double perovskites), and bismuth-based systems (Noel et al., 2014). Scalable deposition techniques compatible with large-area, roll-to-roll manufacturing remain elusive, and the mechanisms governing defect formation, ion migration, and interface recombination in inorganic perovskite devices are still subjects of active investigation.

This review provides a comprehensive and critically evaluated synthesis of the current state of knowledge regarding inorganic perovskite materials for solar cells and optoelectronic applications. It encompasses the fundamental crystal chemistry and electronic

properties of key inorganic perovskite compositions, state-of-the-art fabrication methodologies, device architectures and performance metrics, stability mechanisms and mitigation strategies, applications across the optoelectronic device spectrum, comparative analysis with hybrid organic–inorganic perovskites, environmental and toxicity considerations, and recent advances from 2021–2026. The review concludes with an identification of critical research gaps and a prospective assessment of future directions in the field. By integrating mechanistic insight with device-level analysis, this work aims to provide researchers and engineers with a coherent and actionable understanding of the opportunities and limitations that define the inorganic perovskite landscape.

II. FUNDAMENTALS OF INORGANIC PEROVSKITE MATERIALS

2.1 Crystal Structure and Electronic Properties

The perovskite crystal structure, named after the mineral CaTiO_3 first described by Gustav Rose in 1839, adopts a characteristic ABX_3 framework in which the B-site cation occupies corner-sharing octahedral coordination sites (BX_6 octahedra), while the larger A-site cation resides in 12-fold cuboctahedral coordination within the three-dimensional network of corner-connected octahedra. This structural motif exhibits remarkable compositional flexibility, accommodating a wide range of cation and anion combinations provided that the Goldschmidt tolerance factor (t) falls within the empirically established stability window of approximately $0.8 \leq t \leq 1.0$, where $t = (r_A + r_X) / [\sqrt{2}(r_B + r_X)]$ and r_A , r_B , r_X denote the ionic radii of the respective species (Stranks & Snaith, 2015).

For caesium-based inorganic perovskites, the Cs^+ cation (ionic radius $\sim 1.74 \text{ \AA}$) occupies the A-site, lead (II) (ionic radius $\sim 1.19 \text{ \AA}$) or tin (II) ($\sim 1.18 \text{ \AA}$) occupies the B-site, and the halide anion (I^- : $2.20 \text{ \AA}$, Br^- : $1.96 \text{ \AA}$, Cl^- : $1.81 \text{ \AA}$) occupies the X-site. The tolerance factors of CsPbI_3 , CsPbBr_3 , and CsPbCl_3 are approximately 0.895, 0.918, and 0.938, respectively all within the perovskite stability window. However, for CsPbI_3 , the tolerance factor proximity to the lower boundary renders the cubic (alpha) phase marginally

stable at room temperature, necessitating elevated temperatures or engineered environments to maintain the photoactive phase (Eperon et al., 2015).

Inorganic lead halide perovskites exhibit polymorphism, adopting distinct crystal structures at different temperatures. CsPbI₃, for instance, exists as the cubic alpha-phase ($Pm\bar{3}m$ space group, $E_g \approx 1.73$ eV) above approximately 310°C, transitioning through tetragonal beta and orthorhombic gamma phases upon cooling before reverting to the non-perovskite orthorhombic delta (yellow) phase ($Pnma$ space group, $E_g > 2.8$ eV) at room temperature. The delta phase, characterized by edge-sharing rather than corner-sharing octahedra, is optically inactive for photovoltaic purposes and represents the thermodynamic ground state under ambient conditions. This phase instability is the principal obstacle to the deployment of CsPbI₃ in practical devices (Wang et al., 2019).

The electronic structure of inorganic lead halide perovskites is governed by the hybridization between the Pb 6s and halide p orbitals, forming the valence band maximum, and the Pb 6p orbitals, which predominantly constitute the conduction band minimum. This electronic configuration confers several technologically favorable properties: direct bandgaps spanning the visible spectrum (1.73–2.36 eV for CsPbI₃–CsPbBr₃), high absorption coefficients ($\sim 10^5$ cm⁻¹ at 500 nm), long charge carrier lifetimes (microsecond scale in high-quality films), and large carrier diffusion lengths (hundreds of nanometers to micrometers). The 'defect-tolerant' character of lead halide perovskites arises from the placement of dominant defect states (primarily halide vacancies) near or within the bands rather than deep within the bandgap, minimizing non-radiative recombination (Huang et al., 2017).

2.2 Band Gap Engineering

One of the most powerful attributes of inorganic perovskites is the capacity for continuous and precise bandgap tuning through compositional manipulation. Mixed-halide compositions CsPb(I_xBr_{1-x})₃ and CsPb(Br_xCl_{1-x})₃ enable smooth coverage of the visible spectrum from approximately 1.73 eV to 3.0 eV, making them particularly attractive for spectrally

tailored applications. Vegard's law provides a reasonable approximation of the compositional dependence, though deviations arising from local structural distortions and phase segregation under illumination complicate the picture, especially for iodide-rich mixed-halide compositions (Comin & Sargent, 2016).

Quantum confinement in zero-dimensional (0D) nanocrystals and two-dimensional (2D) nanoplatelets provides an additional dimension of bandgap control beyond compositional tuning. CsPbBr₃ quantum dots (QDs) with diameters below the Bohr exciton radius (~ 7 nm) exhibit size-dependent blue-shifts of up to several hundred meV, enabling emission wavelengths not accessible through bulk compositional engineering alone. The strong quantum confinement also enhances exciton binding energies (to ~ 50 – 100 meV in thin 2D structures), boosting photoluminescence quantum yields (PLQYs) often approaching unity in optimized CsPbBr₃ QD systems and suppressing non-radiative recombination pathways. These properties are particularly exploited in LED and laser applications where high radiative efficiency is paramount (Castañeda et al., 2016; Akkerman et al., 2018).

Strain engineering, achieved through substrate lattice mismatch, mechanical deformation, or compositional gradients, offers yet another modality for bandgap modulation. Compressive or tensile strain alters the Pb–X–Pb bond angles and lengths within the octahedral framework, shifting the band edges and modifying carrier effective masses. Computational studies employing density functional theory (DFT) with hybrid functionals and spin-orbit coupling corrections have provided quantitative predictions of strain-bandgap relationships, informing experimental design strategies for strain-engineered perovskite heterostructures (Huang et al., 2017).

2.3 Charge Transport Properties

The exceptional charge transport characteristics of inorganic perovskites combining large carrier mobilities, long diffusion lengths, and low trap densities are fundamental to their photovoltaic and optoelectronic performance. Time-resolved photoluminescence (TRPL), transient absorption spectroscopy, and Hall effect measurements on

CsPbBr₃ thin films have reported electron and hole mobilities in the range of 1000–4000 cm²V⁻¹s⁻¹ for single crystals (Huang et al., 2017), decreasing to 10–200 cm²V⁻¹s⁻¹ in polycrystalline thin films due to grain boundary scattering. For comparison, single-crystal CsPbI₃ exhibits hole and electron mobilities of approximately 62 and 47 cm²V⁻¹s⁻¹, respectively, consistent with smaller bandwidth arising from its larger bandgap (Fu et al., 2015).

The ambipolar character of charge transport in lead halide perovskites where both electrons and holes exhibit comparable mobilities is advantageous for photovoltaic applications, enabling efficient charge collection from both selective contacts without severe recombination losses. Carrier lifetimes in optimized CsPbI₃ films can exceed several microseconds, translating to diffusion lengths of several micrometers more than sufficient for complete absorption of incident photons within the perovskite absorber layer. However, ion migration, particularly of halide vacancies under applied electric fields, can create space charge regions that limit charge extraction efficiency and contribute to hysteresis in current–voltage (J–V) measurements, a phenomenon more pronounced in inorganic perovskites than in their hybrid counterparts under certain conditions (Kang & Park, 2019).

III. SYNTHESIS AND FABRICATION TECHNIQUES

3.1 Solution-Phase Processing

Solution-phase deposition methods constitute the most widely employed fabrication approach for inorganic perovskite thin films in laboratory-scale device research, owing to their simplicity, low cost, and compatibility with a broad range of substrate geometries. The standard approach involves dissolving stoichiometric quantities of cesium halide (CsX) and lead halide (PbX₂) precursors in polar aprotic solvents such as dimethylformamide (DMF), dimethylsulfoxide (DMSO), or N-methyl-2-pyrrolidinone (NMP), followed by spin-coating onto the substrate and thermal annealing. A critical distinction from hybrid perovskite processing is the requirement for substantially higher annealing temperatures (200–350°C) to drive crystallization of

the inorganic phase and, in the case of CsPbI₃, to access the thermodynamically metastable black phase (Fu et al., 2015).

Antisolvent engineering involving the rapid introduction of a miscible but non-coordinating solvent (e.g., diethyl ether, chlorobenzene, or toluene) during spin-coating to accelerate nucleation and suppress large grain growth has been effectively translated from hybrid to inorganic perovskite processing. The timing, volume, and chemical identity of the antisolvent critically determine film morphology, grain size distribution, and ultimately device performance. Additives introduced into the precursor solution, including ammonium halides, Lewis's acid–base pairs, and organic ligands, play important roles in controlling nucleation kinetics, passivating surface defects, and stabilizing the desired crystalline phase (Xue et al., 2020).

3.2 Vapor-Phase Deposition Methods

Physical vapor deposition (PVD) techniques including thermal evaporation and co-evaporation of CsX and PbX₂ precursors offer significant advantages for large-area, substrate-agnostic deposition with precise thickness control and absence of solvent residues that can introduce undesirable impurities. Dual-source thermal co-evaporation of CsI and PbI₂ at independently controlled rates enables stoichiometry tuning and has been demonstrated to produce highly uniform CsPbI₃ films over areas exceeding 10 cm² with excellent reproducibility. Chemical vapor deposition (CVD) approaches, particularly those utilizing metal-organic precursors in a carrier gas stream, provide an alternative route to conformal coating of complex substrate topographies and have been explored for perovskite nanostructure synthesis. Atomic layer deposition (ALD) and molecular layer deposition (MLD), while not yet widely demonstrated for bulk perovskite film growth, have found application in depositing ultrathin interfacial layers (e.g., Al₂O₃, TiO₂, or self-assembled monolayers) that serve as passivation layers, diffusion barriers, or recombination inhibitors at the perovskite interface with charge transport layers. The integration of vapor-phase deposited inorganic perovskite absorbers with ALD-processed interfacial engineering layers

represents a particularly promising approach to industrially scalable device fabrication.

3.3 Nanocrystal Synthesis

The synthesis of colloidal inorganic perovskite nanocrystals (NCs) enabling quantum-confined optical properties and compatibility with solution-processable device fabrication has evolved substantially from the seminal hot-injection method reported by Protesescu et al. (2015). In this approach, Cs-oleate is rapidly injected into a hot solution (150–200°C) of PbX_2 dissolved in octadecene with coordinating ligands (oleyl amine and oleic acid), inducing rapid nucleation of size-controlled CsPbX_3 NCs. The ligand shell, while critical for colloidal stability and surface passivation, introduces challenges for solid-state film casting and device integration, as the insulating organic ligands impede interparticle charge transport.

Post-synthetic ligand exchange strategies replacing bulky native ligands with shorter, more conductive alternatives such as methylammonium iodide, formamidinium iodide, or inorganic ligands (e.g., sulfide, iodide) have substantially improved carrier mobility in NC films and enabled higher-performance optoelectronic devices. Phase transfer ligand exchange protocols, in which NCs dispersed in non-polar media are transferred to more polar solvents compatible with subsequent processing, have further expanded the integration possibilities. Room-temperature synthesis methods, including reprecipitation and ultrasonication-assisted techniques, provide scalable alternatives to hot-injection for gram-scale production, though often at the expense of size distribution uniformity.

3.4 Advanced Fabrication: Printing and Scalable Methods

The transition from laboratory-scale spin-coating to industrially relevant deposition methods is a prerequisite for commercialization. Slot-die coating, blade coating, inkjet printing, and screen printing have all been demonstrated for inorganic perovskite film deposition, with varying degrees of film quality. Blade-coating of CsPbI_2Br precursor solutions has yielded device PCEs exceeding 16% on areas of 1 cm^2 , approaching spin-coated benchmarks. However,

controlling the crystallization dynamics during high-speed deposition over large areas where solvent evaporation rates, temperature gradients, and film thickness uniformity must be simultaneously managed remains a significant engineering challenge.

IV. INORGANIC PEROVSKITES IN SOLAR CELL APPLICATIONS

4.1 Device Architectures

Inorganic perovskite solar cells are typically constructed in either n-i-p (conventional) or p-i-n (inverted) planar architectures, with the choice of structure influencing the charge transport layer (CTL) selection, processing compatibility, and hysteresis behavior. In the n-i-p architecture, electrons flow from the perovskite absorber through an electron transport layer (ETL), commonly TiO_2 (compact and/or mesoporous), SnO_2 , or ZnO , to the transparent conducting oxide (TCO, typically fluorine-doped tin oxide, FTO) back contact. Holes are extracted through a hole transport layer (HTL) historically Spiro-OMeTAD, but increasingly inorganic HTLs such as CuSCN , NiO_x , CuI , or Cu_2O for enhanced thermal compatibility to the metal back electrode (typically gold or silver) (Chen et al., 2015).

The p-i-n (inverted) architecture places the HTL adjacent to the transparent front electrode, with the perovskite absorber sandwiched between the HTL and ETL before the metal back contact. Poly(3,4-ethylenedioxythiophene): polystyrene sulfonate (PEDOT: PSS) has been widely used as the HTL in inverted architectures, though its acidity and hygroscopicity are concerns. Inorganic alternatives including NiO_x and CuSCN offer improved stability. The inverted architecture is generally associated with lower hysteresis indices and compatibility with lower processing temperatures, making it attractive for flexible and tandem device applications (Stranks & Snaith, 2015).

4.2 Champion Efficiency Milestones

CsPbI_2Br (bandgap $\sim 1.92\text{ eV}$) has emerged as the most studied binary mixed-halide inorganic perovskite for single-junction photovoltaics, offering a favorable compromise between phase stability and bandgap suitability. Certified PCEs for CsPbI_2Br devices have

progressively improved from below 10% in 2016–2017 to values exceeding 17–18% in recent reports from leading groups (Jiang et al., 2019; Liu et al., 2021; Wang et al., 2022). For the more challenging but more bandgap-optimal CsPbI₃ (E_g ~1.73 eV), careful phase stabilization strategies have enabled champion PCEs approaching 20–21% in research settings (Swarnkar et al., 2016; Wang et al., 2019; Zhao et al., 2022; Zhou et al., 2023).

The efficiency of CsPbBr₃ single-junction cells is fundamentally constrained by its relatively wide bandgap (~2.36 eV), which limits the photocurrent density achievable under the AM1.5G solar spectrum.

Maximum theoretical PCEs of ~12% are predicted by Shockley–Queisser analysis for this bandgap; experimentally, certified efficiencies of 10–11% have been reported. Nevertheless, CsPbBr₃ offers exceptional thermal and atmospheric stability that makes it attractive for specific niche applications and as a top cell in all-perovskite tandem configurations. Lead-free alternatives, including CsSnI₃-based devices and Cs₂AgBiBr₆ double perovskite cells, have achieved PCEs of 14% and 4–6%, respectively, as of 2024–2025 substantially below their lead-based counterparts but showing consistent improvement (Kulbak et al., 2015).

Table 1. Performance Summary of Representative Inorganic Perovskite Solar Cell Devices (2019–2025)

Material	E _g (eV)	J _{sc} (mA/cm ²)	V _{oc} (V)	FF (%)	PCE (%)	Reference
CsPbI ₂ Br	1.92	15.6	1.23	79.4	18.0	(Wang et al., 2022)
CsPbI ₃ (NC)	1.73	17.3	1.25	78.8	20.1	(Zhao et al., 2022)
CsPbBr ₃	2.36	7.8	1.51	83.1	9.8	(Kulbak et al., 2016)
CsPbI ₂ Br (blade)	1.92	15.1	1.19	76.2	16.4	(Liu et al., 2021)
CsSnI ₃	1.30	22.1	0.88	72.3	14.1	(Chung et al., 2023)
Cs ₂ AgBiBr ₆	1.95	3.2	1.22	65.0	6.4	(Greul et al., 2017)

4.3 Interface Engineering and Defect Passivation

Interfaces between the perovskite absorber and charge transport layers represent critical junctures where non-radiative recombination, band misalignment, and interfacial ionic accumulation collectively limit device performance. At the perovskite/ETL interface (typically perovskite/TiO₂ or perovskite/SnO₂), undercoordinated Pb²⁺ ions, halide vacancies, and surface oxygen species create trap states that can facilitate Shockley–Read–Hall (SRH) recombination, reducing open-circuit voltage (V_{oc}) below the radiative limit. Passivation strategies targeting these interfacial defects have produced some of the most significant efficiency gains in recent literature (Jiang et al., 2019).

Molecular passivation agents including Lewis bases with lone-pair electron donors (e.g., pyridine derivatives, thiophene compounds, and various amine and thiol functionalities), Lewis’s acids that

compensate surface anion vacancies, and bifunctional organic molecules that bridge the perovskite surface and CTL have been demonstrated to reduce trap state densities by up to two orders of magnitude in optimized systems. The introduction of thin interlayers of alkali metal halides (e.g., KI, RbBr, or LiF) at the perovskite/CTL interfaces, exploiting the propensity of alkali ions to segregate to surfaces and grain boundaries, has proven particularly effective for suppressing interface recombination while simultaneously improving band alignment (Liu et al., 2023).

Grain boundary passivation within the perovskite absorber bulk is equally critical, as grain boundaries in polycrystalline thin films concentrate defects and provide pathways for preferential ion migration. Post-deposition treatments using methylammonium iodide, formamidinium bromide vapor, or solution-phase treatments with guanidinium thiocyanate have been

shown to rectify grain boundary defects and improve long-range compositional homogeneity in inorganic perovskite films. Particularly innovative is the use of in situ-forming passivation agents that are generated during thermal annealing from embedded precursors, enabling concurrent grain growth and defect passivation in a single processing step (Xue et al., 2020).

V. STABILITY CHALLENGES AND DEGRADATION MECHANISMS

5.1 Phase Instability

The thermodynamic instability of the photoactive perovskite phase in inorganic cesium lead iodide compositions represents the most fundamental obstacle to device lifetime. CsPbI₃, with its tolerance factor of ~0.895, occupies a marginal stability region where the cubic black phase is thermodynamically favored only at elevated temperatures (above ~310°C at ambient pressure). Upon cooling below this transition temperature, the free energy landscape favors the non-perovskite orthorhombic delta phase, in which PbI₆ octahedra share edges rather than corners, completely disrupting the electronic band structure favorable for photovoltaic operation (Eperon et al., 2015).

The kinetics of the black-to-yellow phase transformation are highly sensitive to environmental conditions: humidity, oxygen concentration, temperature cycling, and illumination intensity all accelerate the phase transition. Water vapor is particularly deleterious, as it can both dissolve the cesium halide framework and catalyze the phase transformation by reducing the activation energy for structural rearrangement. Under rigorously controlled inert atmosphere and dry conditions, black-phase CsPbI₃ thin films can remain kinetically stable at room temperature for extended periods; however, any exposure to ambient conditions substantially accelerates degradation (Swarnkar et al., 2016).

5.2 Moisture and Oxygen Degradation

Beyond phase instability, moisture and oxygen act as primary chemical degradation agents in inorganic perovskite films. The hydrolysis of CsPbI₃ proceeds through the formation of Cs₄PbI₆·H₂O hydrate

intermediates, ultimately decomposing to CsI, PbI₂, and iodine gas. While inorganic perovskites exhibit substantially higher intrinsic moisture resistance than methylammonium-based HOIPs (due to the absence of the readily hydrolyzed C–N bonds), their stability remains insufficient for outdoor deployment without robust encapsulation. Oxygen, in conjunction with light, can oxidize Pb²⁺ and iodide species, generating superoxide radicals that propagate degradation through a chain mechanism (Zhao et al., 2022).

CsPbBr₃, with its smaller, more electronegative bromide anion and correspondingly stronger Cs–Br and Pb–Br bonding, exhibits substantially superior moisture and oxygen stability compared to CsPbI₃. CsPbBr₃ quantum dot films have been reported to retain >95% of their photoluminescence intensity after prolonged exposure to 50% relative humidity, while CsPbI₃ films under similar conditions degrade within hours. This stark contrast in ambient stability between bromide and iodide compositions reflects both the thermodynamic stability of the crystalline phase and the kinetics of halide vacancy formation and migration (Kulbak et al., 2016).

5.3 Thermal Stability

A defining advantage of inorganic perovskites over their hybrid counterparts is thermal stability. While MAPbI₃ decomposes at temperatures exceeding ~150°C through volatile methylamine evolution, CsPbI₃ and CsPbBr₃ can withstand temperatures of 300–400°C before significant decomposition occurs, as evidenced by thermogravimetric analysis (TGA) and in situ X-ray diffraction studies. This enhanced thermal durability enables compatibility with high-temperature device fabrication processes, including those used in silicon-perovskite tandem cell manufacturing. However, repeated thermal cycling as experienced during actual outdoor solar cell operation can promote additional degradation through differential thermal expansion between the perovskite absorber and charge transport layers, leading to delamination and microcracking (Huang et al., 2017).

5.4 Ion Migration

Ion migration, particularly of halide anions and their vacancies under the influence of electric fields and thermal gradients, is a pervasive phenomenon in metal

halide perovskites that contributes to hysteresis in J–V characteristics, slow response dynamics, and long-term degradation. Activation energies for halide ion migration in lead halide perovskites are typically in the range of 0.1–0.5 eV, implying significant mobility at room temperature and above. In inorganic perovskites, ion migration is exacerbated by the absence of bulky organic spacers (as found in 2D Ruddlesden–Popper

phases) that can impede ionic diffusion. The migration of iodide ions toward the illuminated interface under sustained operation can create iodide-depleted regions with modified band structure, contributing to device performance degradation over time (Kang & Park, 2019).

Table 2. Stability Comparison: Inorganic vs. Hybrid Perovskites Under Various Degradation Conditions

Degradation Factor	CsPbBr ₃	CsPbI ₂ Br	CsPbI ₃	MAPbI ₃
Thermal (>150°C)	Excellent (>350°C)	Good (~300°C)	Good (~310°C)	Poor (~150°C)
Moisture (RH 50%)	Good (>1000 h)	Moderate (~500 h)	Poor (<100 h)	Poor (<24 h)
UV Illumination	Good	Moderate	Poor–Moderate	Poor
Phase Stability (RT)	Excellent	Good	Poor (delta phase)	Good
Oxygen	Good	Moderate	Moderate	Poor

VI. STRATEGIES FOR IMPROVING STABILITY AND EFFICIENCY

6.1 Compositional Engineering

Compositional engineering through multi-cation and multi-anion alloying has emerged as the most versatile strategy for simultaneously addressing phase stability and band gap optimization in inorganic perovskites. Partial substitution of Pb²⁺ with smaller divalent cations including Sn²⁺, Mn²⁺, Cd²⁺, and Sr²⁺ modifies octahedral tilting, lattice parameters, and tolerance factors in ways that can stabilize the black phase. For example, partial Mn²⁺ incorporation into CsPbI₃ at levels of 5–15 mol% has been demonstrated to suppress the delta-phase transition while simultaneously improving carrier mobility and reducing defect density (Swarnkar et al., 2016).

Heterovalent doping with lanthanide cations (La³⁺, Sm³⁺, Yb³⁺) has attracted attention both for phase stabilization and for enabling energy transfer-based spectral conversion, where high-energy photons absorbed by the perovskite host are down-converted to near-infrared emission matching the absorption maximum of silicon an effect potentially exploitable in silicon-perovskite tandem architectures. Bismuth (Bi³⁺) doping modifies the electronic structure while improving thermal stability, though careful

optimization is required to avoid the introduction of deep trap states that accompany excessive Bi incorporation.

6.2 Surface and Grain Boundary Passivation

As discussed in Section 4.3, targeted passivation of surface and grain boundary defects is among the most impactful strategies for improving both efficiency and stability. Beyond molecular Lewis acid–base passivation, recent innovations include: (i) atomic-layer-deposited encapsulation shells of Al₂O₃ or SiO₂ that simultaneously passivate surface trap states and retard moisture ingress; (ii) pseudo-halide anion (e.g., thiocyanate SCN[−], formate HCOO[−]) incorporation that replaces halide vacancies with more stable anions having similar ionic radii; and (iii) self-assembled monolayer (SAM) interlayers at the perovskite/CTL interface that combine defect passivation with improved energy level alignment (Shi et al., 2018).

6.3 Dimensionality Reduction and 2D–3D Heterostructures

Two-dimensional (2D) Ruddlesden–Popper perovskites, with the general formula L₂Cs_{n-1}Pb_nX_{3n+1} (where L is a long-chain organic ammonium spacer cation), exhibit dramatically enhanced moisture and phase stability compared to

their three-dimensional counterparts, attributable to the hydrophobic organic spacer layers that retard water infiltration. However, the quantum confinement imposed by the 2D structure increases exciton binding energies and reduces carrier mobilities along the out-of-plane direction, limiting charge extraction efficiency in photovoltaic devices. Vertically oriented 2D perovskite phases with favorable out-of-plane carrier transport, achieved through careful crystallization control, represent a strategy to capture the stability benefits of 2D structures while preserving photovoltaic efficiency (Chen et al., 2018).

Compositionally graded 2D–3D heterostructures in which a thin 2D perovskite capping layer is formed at the surface of a 3D perovskite bulk by post-deposition treatment with spacer organic ammonium solutions combine the photovoltaic efficiency of the 3D bulk with the surface stability of the 2D layer. This 'quasi-2D' or '3D/2D bilayer' approach has produced significant improvements in both stability and efficiency in numerous published studies, with several groups reporting T80 lifetimes (time to 80% of initial PCE) exceeding 1000 hours under simulated 1-sun illumination without encapsulation (Chen et al., 2018).

6.4 Encapsulation Technologies

Device-level encapsulation provides the first line of defense against environmental degradation independent of the intrinsic stability of the perovskite material. Glass-glass lamination with ethylene vinyl acetate (EVA) or polyolefin elastomer (POE) interlayers, borrowed directly from silicon PV module technology, has been demonstrated to dramatically extend inorganic perovskite device lifetimes under standard IEC 61215 test conditions (damp heat, UV exposure, thermal cycling). Edge sealants with ultra-low water vapor transmission rates (WVTR < 10⁻⁵ g/m²/day) are critical to preventing moisture ingress through module perimeters. Atomic-layer-deposited barrier coatings (Al₂O₃, ZnO, TiO₂, or their composites) applied conformally over device surfaces provide an additional moisture barrier layer compatible with thin-film and flexible device formats (Filonenko et al., 2024).

VII. APPLICATIONS IN OPTOELECTRONIC DEVICES

7.1 Light-Emitting Diodes (LEDs)

Inorganic perovskite LEDs (PeLEDs) have witnessed remarkable efficiency improvements, driven by the exceptional photoluminescence quantum yields (PLQYs) achievable in CsPbBr₃ and CsPbX₃ nanocrystal systems. The key optoelectronic metrics of a PeLED external quantum efficiency (EQE), luminance, current efficiency (CE), and operational lifetime are collectively determined by the radiative recombination rate within the emitter layer, the charge injection balance from the CTLs, and the light out-coupling efficiency of the device architecture. CsPbBr₃ nanocrystal LEDs have achieved EQEs exceeding 22% in optimized laboratory devices (Ling et al., 2023), approaching the theoretical limit for planar architectures and comparable to state-of-the-art organic LEDs (OLEDs) in the green emission range (Tan et al., 2014; Zhao et al., 2018).

Red-emitting CsPbI₃ and CsPb(I/Br)₃ nanocrystal LEDs present greater challenges owing to the phase instability of iodide-rich compositions under applied electric fields and elevated current densities, which can drive halide ion migration and spectral blue-shifting during device operation. Strategies including composition optimization (maintaining Br content above a critical threshold), passivation with multifunctional ligands, and device architecture engineering (thin emitter layers to minimize ion migration pathways) have progressively improved the operational stability of red PeLEDs. Narrow spectral emission (full-width at half-maximum < 20 nm for green CsPbBr₃) combined with wide color gamut coverage (exceeding Rec. 2020 standards) makes inorganic perovskite emitters particularly attractive for display technology applications (Jiang et al., 2022).

7.2 Photodetectors

The combination of high carrier mobility, large absorption coefficients, and low trap densities in inorganic perovskite single crystals and thin films translates directly into exceptional photodetector performance. CsPbBr₃ and CsPbI₃ single-crystal photodetectors have demonstrated specific detectivities (D*) exceeding 10¹³ Jones, response

times in the nanosecond to microsecond range (depending on device geometry and carrier transit time), and linear dynamic ranges (LDRs) exceeding 100 dB performance metrics that compare favorably with commercial silicon photodiodes across broad spectral ranges. The high X-ray absorption cross-section of lead in CsPbBr₃ ($Z_{\text{Pb}} = 82$) makes inorganic perovskites particularly attractive for ionizing radiation detection, with demonstrated sensitivity values of $>100 \mu\text{C Gy}^{-1} \text{cm}^{-2}$ for direct X-ray conversion several orders of magnitude superior to amorphous selenium detectors (Gao et al., 2016).

Self-powered photodetectors based on inorganic perovskite p–n or p–i–n junctions, which operate without external bias by utilizing the photovoltaic effect for charge separation, have been extensively reported for CsPbBr₃ and CsPbI₂Br systems. These devices are of particular interest for IoT sensor applications where energy autonomy is desirable. The spectral tunability of inorganic perovskites through halide engineering enables the realization of photodetectors optimized for specific wavelength windows in UV, visible, and near-infrared ranges (Fu et al., 2015).

7.3 Lasers and Optical Gain Media

The combination of large absorption oscillator strengths, narrow emission linewidths, and low non-radiative recombination rates makes inorganic perovskites highly promising gain media for optically pumped laser applications. Amplified spontaneous emission (ASE) the precursor to lasing has been observed in CsPbBr₃ nanocrystal films with threshold fluences as low as a few $\mu\text{J cm}^{-2}$ under femtosecond pulsed excitation (Yakunin et al., 2015), reflecting the high optical gain coefficients ($>100 \text{cm}^{-1}$) attainable in optimized inorganic perovskite emitter layers. Whispering gallery mode (WGM), distributed feedback (DFB), and vertical cavity surface-emitting laser (VCSEL) configurations have all been demonstrated using inorganic perovskite gain layers (Zhu et al., 2015).

Progress toward electrically driven lasing in inorganic perovskite devices the ultimate goal for practical laser applications has been impeded by the challenge of simultaneously achieving the high current densities

required for population inversion while maintaining low non-radiative recombination rates and preventing Joule heating-induced degradation. The demonstration of low-threshold optical gain in continuous-wave (CW) excitation conditions, a prerequisite for practical CW laser operation, remains a key research milestone yet to be convincingly demonstrated in inorganic perovskite systems as of 2025.

7.4 Sensors and Other Applications

Beyond photovoltaics and traditional optoelectronics, inorganic perovskites are finding application as chemical and physical sensors exploiting their sensitivity to environmental perturbations. CsPbBr₃ nanocrystals have been demonstrated as luminescent humidity sensors, ion sensors (particularly for anions that undergo halide exchange reactions with the perovskite surface), and temperature sensors (exploiting the temperature-dependent shift in emission wavelength with sensitivities of $\sim 0.1\text{--}0.3 \text{nm/}^\circ\text{C}$). Pressure-sensitive perovskite devices exploiting piezoresistive or piezoluminescent phenomena have also been reported (Shi et al., 2018). Inorganic perovskite scintillators for high-energy radiation detection represent a particularly exciting emerging application. CsPbBr₃ and Cs₂AgBiBr₆ single crystals have demonstrated scintillation light yields and energy resolutions competitive with established commercial scintillators such as NaI(Tl) and CsI(Tl) for gamma-ray detection, with the added advantage of low-cost, solution-processable production. The integration of inorganic perovskite scintillators with amorphous silicon or IGZO thin-film transistor readout arrays is being actively explored for flat-panel X-ray imaging detector applications (Greul et al., 2017).

VIII. COMPARATIVE ANALYSIS: INORGANIC VS. HYBRID ORGANIC–INORGANIC PEROVSKITES

A rigorous comparative analysis of all-inorganic and hybrid organic–inorganic perovskites (HOIPs) reveal a multidimensional trade-off landscape in which no single material system dominates across all performance metrics. HOIPs, particularly formamidinium lead iodide (FAPbI₃) and its caesium/rubidium co-doped derivatives, have

achieved the highest certified PCEs for single-junction perovskite solar cells (>26% as of 2025), benefiting from near-ideal bandgap (~1.47–1.55 eV for FA-rich compositions) and superior charge carrier properties relative to most inorganic compositions. The inclusion of organic FA or MA cations, however, introduces inherent thermodynamic instability: decomposition temperatures below 200°C, hygroscopic degradation within hours under ambient exposure, and phase segregation under illumination collectively limit practical device lifetimes (Chen et al., 2015).

All-inorganic perovskites sacrifice some photovoltaic efficiency primarily through somewhat wider, less

optimal bandgaps in exchange for substantially superior thermal and moisture stability. The operational stability demonstrated by encapsulated inorganic perovskite solar cells under IEC 61215-equivalent thermal cycling (−40°C to +85°C) and damp heat (85°C, 85% RH) protocols significantly exceeds that of unencapsulated HOIPs, though properly encapsulated HOIP devices can also achieve impressive lifetimes. The distinction becomes most relevant for high-temperature deployment environments and for applications requiring low-cost encapsulation without hermetic sealing (Filonenko et al., 2024).

Table 3. Comparative Properties: Key Inorganic vs. Hybrid Perovskite Compositions

Property	CsPbI ₂ Br	CsPbBr ₃	FAPbI ₃	MAPbI ₃	Note
Bandgap (eV)	1.92	2.36	1.47	1.55	Tunable via halide mixing
Best PCE (%)	~18	~10	~26.1	~23	Certified, single junction
Thermal stability	Good	Excellent	Moderate	Poor (<150°C)	Decomposition onset
Moisture stability	Moderate	Good	Poor	Very poor	Without encapsulation
PLQY	High (up to 90%)	Very high (>95%)	High (~80%)	Moderate (~60%)	In optimized nanocrystals
Phase stability (RT)	Good	Excellent	Moderate	Good	Ambient air, no encapsulation
Lead content	Yes	Yes	Yes	Yes	Environmental concern

From an optoelectronics perspective beyond photovoltaics, inorganic perovskites hold clear advantages in high-temperature LED applications (e.g., automotive and industrial lighting), where the inability of organic cations to withstand sustained high-temperature operation limits HOIP deployment. In contrast, HOIPs particularly low-dimensional 2D compositions can achieve broader tunability of emission color and linewidth through organic spacer cation engineering, which remains challenging to replicate in purely inorganic systems (Adjokatse et al., 2017).

IX. ENVIRONMENTAL, TOXICITY, AND SCALABILITY CONSIDERATIONS

9.1 Lead Toxicity and Regulatory Context

The pervasive use of lead in high-performance inorganic perovskites raises fundamental questions regarding environmental safety, regulatory compliance, and lifecycle sustainability. Lead is a well-documented neurotoxin with severe developmental consequences, particularly in children, and its use is restricted under multiple international regulatory frameworks including the European Union's Restriction of Hazardous Substances

Directive (RoHS) and the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) regulations. While photovoltaic panels are currently partially exempted from RoHS restrictions, this exemption is subject to ongoing review and may not be maintained as perovskite technology approaches commercialization (Noel et al., 2014).

Quantitative lifecycle assessment (LCA) studies of perovskite solar modules have generally concluded that the lead content in a typical perovskite PV panel (approximately 0.5–1 g/m²) is comparable to or lower than the lead content in conventional lead-acid batteries used in off-grid solar installations, and substantially below the regulatory thresholds that would trigger immediate restriction under current frameworks. However, the water solubility of lead iodide and methylammonium lead iodide decomposition products under outdoor weathering conditions raises concerns about environmental contamination during module failure or end-of-life disposal, necessitating robust encapsulation and recycling protocols. Kang and Park (2019) estimated that a 2% global electricity generation scenario based on perovskite PV could release approximately 2,500 tons of lead annually under uncontrolled degradation conditions a figure that underscores the urgency of developing water-stable encapsulants and lead-containing recycling systems.

9.2 Lead-Free Alternatives

The development of lead-free inorganic perovskites and perovskite-inspired materials represents an active and growing research priority. Tin-based perovskites (CsSnI₃, CsSnBr₃, Cs₂SnI₆) offer the most direct isoelectronic substitution for lead, with comparable or superior bandgaps and potentially high carrier mobilities. However, the facile oxidation of Sn²⁺ to Sn⁴⁺ under ambient conditions introduces a self-doping effect that dramatically increases non-radiative recombination and reduces device open-circuit voltage. Rigorous air-free processing environments and the use of reducing agent additives (e.g., SnF₂, hydrazine) have partially mitigated Sn²⁺ oxidation, enabling CsSnI₃-based solar cells with PCEs approaching 14% under optimized conditions (Li et al., 2021).

Double perovskites (elpasolites) with the formula Cs₂B'B''X₆, where B' is a monovalent cation (e.g., Ag⁺, Na⁺) and B'' is a trivalent cation (e.g., Bi³⁺, Sb³⁺, In³⁺), completely avoid lead while maintaining the perovskite structural framework. Cs₂AgBiBr₆ is the most extensively studied member of this family, with an indirect bandgap of ~1.95 eV and demonstrated photovoltaic PCEs of 4–6%. The indirect bandgap, arising from the momentum mismatch between the valence band maximum (dominated by Ag 4d and Br 4p states) and the conduction band minimum (Bi 6p character), fundamentally limits the absorption coefficient and short-circuit current density attainable. Strategies to overcome the indirect gap limitation including alloying with in-gap-state-forming cations, defect engineering to create disorder-activated optical transitions, and quantum dot dimensionality reduction are active research directions (Greul et al., 2017).

Bismuth-based perovskite-inspired materials, including Cs₃Bi₂I₉, Cs₃Bi₂Br₉, and related vacancy-ordered perovskites (with the general formula A₃B₂X₉), have attracted interest for their intrinsic stability and non-toxic composition, but suffer from very wide bandgaps (>2.0 eV) and low carrier mobilities due to structural distortions associated with the vacancy ordering. Antimony-based (Sb³⁺) analogues exhibit similar challenges. Progress in these systems has been most notable in optoelectronic applications where high efficiency is not the primary metric particularly for stable photo(electro)catalysis, radiation detection, and luminescence applications (Noel et al., 2014).

9.3 Scalability and Manufacturing Challenges

The transition from laboratory-scale (0.1 cm²) champion devices to module-scale (>100 cm²) products introduces a set of engineering challenges that are distinct from those encountered in fundamental materials optimization. Film uniformity over large areas is critically dependent on the uniformity of substrate temperature, solvent evaporation rate, and precursor concentration parameters that are straightforward to control in spin-coating but become progressively more difficult to manage in scalable deposition methods. Current density and voltage non-uniformity across large-area modules, arising from sheet resistance of the TCO

layer and lateral current collection constraints, require optimized interconnect geometries (typically P1/P2/P3 laser scribing) to minimize active area losses.

The hygroscopic and air-sensitive nature of most inorganic perovskite precursor solutions necessitates controlled-atmosphere manufacturing environments, adding capital expenditure costs. Life-cycle cost analyses suggest that the key drivers of perovskite module manufacturing cost will be the throughput of deposition equipment, raw material costs (particularly specialty solvents and hole transport materials), and yield the latter being particularly sensitive to particle contamination and substrate surface quality in high-speed deposition processes.

X. RECENT ADVANCES AND EMERGING TRENDS (2021–2026)

10.1 Efficiency Breakthroughs

The period from 2021 to 2026 has been characterized by sustained efficiency improvement in inorganic perovskite solar cells, accompanied by increasingly sophisticated mechanistic understanding of device physics. Notably, Wang et al. (2022) reported a certified PCE of 18.64% for CsPbI₂Br devices employing a multifunctional surface treatment combining a Lewis base passivation agent with an inorganic HTL, demonstrating that the historical efficiency gap between inorganic and hybrid perovskite cells can be substantially narrowed through careful interface engineering. Zhou et al. (2023) demonstrated CsPbI₃ devices with PCEs exceeding 20% through a phase-stable all-inorganic device architecture employing A-site-alloyed CsRb-PbI₃ absorbers with sub-nanometer interlayer passivation (Liu et al., 2023).

Tandem photovoltaic architectures have received particular attention, with all-perovskite two-terminal (2T) tandems combining a wide-bandgap inorganic top cell (CsPbI₂Br or CsPbBr₃, ~1.9–2.4 eV) with a narrow-bandgap tin-lead perovskite bottom cell (~1.2 eV) achieving certified PCEs of 27–28% in 2023–2024, surpassing the single-junction silicon cell efficiency record and approaching the theoretical optimum for a two-junction tandem under AM1.5G

illumination. Perovskite-silicon monolithic tandems incorporating an inorganic top cell have further demonstrated efficiencies approaching 33%, the highest certified values for any perovskite-containing architecture.

10.2 Machine Learning and High-Throughput Screening

The application of machine learning (ML) and artificial intelligence (AI) methodologies to inorganic perovskite materials discovery has accelerated the identification of novel compositions, optimal processing conditions, and stability-enhancing additives beyond what is accessible through traditional trial-and-error experimentation. Graph neural networks trained on high-throughput DFT datasets have demonstrated the capacity to predict formation energies, bandgaps, and phase stability indices for unexplored double perovskite compositions with accuracy approaching that of DFT calculations but at a fraction of the computational cost. Bayesian optimization protocols applied to multi-dimensional perovskite processing parameter spaces have identified optimal spin-coating, antisolvent, and annealing protocols for CsPbI₂Br, reducing the experimental workload for process optimization by approximately 60–80% relative to conventional one-factor-at-a-time approaches (Yuan et al., 2024).

High-throughput experimental platforms, including robotic synthesis systems capable of autonomously preparing, characterizing, and optimizing hundreds of perovskite film and device compositions per day, have been deployed at several leading research institutions and national laboratories. The combination of these autonomous experimental platforms with ML-guided experimental design constitutes a self-improving 'closed-loop' discovery engine that is fundamentally transforming the pace of materials innovation in the inorganic perovskite field (Yuan et al., 2024).

10.3 Advances in Nanocrystal Engineering

Nanocrystal engineering of inorganic perovskites has seen several major advances during 2021–2026. The development of 'ligand-assisted reprecipitation' and continuous flow synthesis methods has enabled gram-scale production of monodisperse CsPbBr₃ quantum dots with PLQYs consistently exceeding 90%,

addressing a key barrier to industrial-scale LED production. Novel ligand engineering strategies including the use of zwitterionic ligands, metal-organic framework (MOF) shell coatings, and amphiphilic block copolymer matrices have demonstrated dramatic improvements in QD colloidal stability and resistance to aggregation-induced quenching in solid-state films (Zhang et al., 2016).

The discovery of 'A-site vacancy' ordered perovskites such as Cs_2PbI_3 and their halide variants as stable, solution-processable quantum well analogues has opened new avenues for emission color control with inherently superior phase stability compared to bulk 3D compositions. Core-shell NC architectures, in which a CsPbBr_3 or CsPbI_3 perovskite core is overcoated with a wider-bandgap inorganic shell (e.g., CsPbCl_3 , Cs_4PbBr_6) through epitaxial or pseudo-epitaxial growth, have been shown to dramatically enhance PLQY and operational photostability, advancing the prospects for practical display and LED applications (Akkerman et al., 2018).

10.4 Flexible and Wearable Devices

The compatibility of inorganic perovskites with low-temperature (below 150°C) processing achieved through careful solvent engineering, UV-ozone substrate treatment, and nanocrystal ink formulations has enabled the fabrication of flexible perovskite photovoltaic and optoelectronic devices on polymer substrates including PET, PEN, and polyimide. Flexible CsPbI_2Br solar cells on PET substrates with PCEs exceeding 15% and retention of >90% initial PCE after 1000 bending cycles (bending radius 5 mm) have been reported, demonstrating the mechanical durability required for wearable energy harvesting applications. Stretchable perovskite photodetectors and LEDs, incorporating micro-structured elastomeric substrates that accommodate large strains through controlled buckling of rigid active-layer islands, represent emerging devices for skin-interfaced health monitoring applications.

XI. FUTURE PROSPECTS AND RESEARCH DIRECTIONS

The trajectory of inorganic perovskite research suggests several transformative developments on the

near-to-medium term horizon. The following research directions are identified as critical priorities for advancing the field toward commercial viability and broader technological impact.

11.1 Phase Stabilization of CsPbI_3

Achieving reliable room-temperature phase stabilization of the black-phase CsPbI_3 with the high efficiency and manufacturability required for commercial deployment remains the 'holy grail' of inorganic perovskite photovoltaics. Promising avenues include: (i) ultrathin (sub-monolayer) ALD-deposited inorganic passivation shells that kinetically trap the black phase by creating an energy barrier to the black-to-yellow phase transition; (ii) porous or strained substrate templates that impose favorable mechanical boundary conditions on the perovskite film; (iii) co-crystallized molecular guests (e.g., crown ethers, calixarenes) that stabilize the Cs^+ coordination environment within the black-phase lattice; and (iv) nanoscale embedding of CsPbI_3 within stable mesoporous oxide scaffolds that physically constrain phase transformation (Swarnkar et al., 2016).

11.2 Genuine Lead-Free High-Efficiency Perovskites

The identification of lead-free inorganic perovskite or perovskite-inspired compositions capable of achieving PCEs above 15% comparable to established thin-film technologies such as CdTe and CIGS is a paramount environmental and regulatory imperative. Computational screening of the enormous compositional space of double perovskites, vacancy-ordered perovskites, and other B-site heterovalent configurations has identified several promising candidates beyond the well-studied $\text{Cs}_2\text{AgBiBr}_6$, including $\text{Cs}_2\text{InAgCl}_6$ (predicted direct bandgap), $\text{Cs}_2\text{TlBiBr}_6$, and various Sb^{3+} -containing analogues. Experimental realization of the theoretically predicted properties of these materials overcoming synthesis challenges related to the precise control of B-site cation ordering and halide stoichiometry is a key near-term research challenge (Greul et al., 2017).

11.3 Tandem and Multi-Junction Architectures

All-inorganic perovskite cells as top-cell components in multi-junction tandems with silicon, CIGS, organic PV, or narrow-bandgap perovskite bottom cells are poised to enable module efficiencies substantially

exceeding the Shockley–Queisser limit for single-junction devices (~33% under concentration). The realization of 30%+ efficiency 4-terminal (4T) and 2-terminal (2T) tandem modules incorporating inorganic perovskite top cells requires the simultaneous optimization of bandgap (matching the two-junction optimal value near 1.73–1.9 eV for a silicon bottom cell), optical transparency of auxiliary layers, tunnel junction or recombination layer conductivity and stability, and monolithic interconnect integration. Progress in laser-scribed monolithic integration and plasma-cleaned interface engineering is rapidly narrowing the efficiency gap between laboratory-scale and module-scale tandem devices.

11.4 Autonomous Discovery and Materials Informatics

The integration of autonomous experimental platforms with physics-informed ML models trained on expanding databases of perovskite properties is expected to accelerate materials discovery at a rate far exceeding traditional research approaches. Crucially, the next generation of ML models for perovskite research must go beyond property prediction to include prediction of degradation mechanisms, encapsulation effectiveness, and processability capturing the full complexity of the stability efficiency processability design space that governs real-world device performance. Open-access databases consolidating crystallographic, optoelectronic, and stability data from the global perovskite research community will be essential infrastructure for realizing the full potential of data-driven materials science in this field (Yuan et al., 2024).

11.5 Commercialization Roadmap

Commercial deployment of inorganic perovskite solar modules is anticipated in niche markets (building-integrated PV, agrivoltaics, specialty electronics) within 5–7 years, contingent on demonstrating T80 lifetimes exceeding 25 years under realistic outdoor conditions a target currently not met by any perovskite system without optimization. The pathway to utility-scale deployment requires the concurrent development of: (i) stable, non-lead or low-lead absorber compositions meeting regulatory standards; (ii) encapsulation systems certified under IEC 61215 and IEC 61646; (iii) scalable deposition methods with

demonstrated yield and uniformity on >1 m² substrates; and (iv) end-of-life recycling infrastructure that recovers and safely manages lead-containing components. Government and private sector investments in perovskite pilot manufacturing lines particularly in China, Europe, and the United States are accelerating this transition, and the first commercial perovskite modules are expected to reach market within the current decade (Filonenko et al., 2024).

XII. CONCLUSION

This review has presented a comprehensive analysis of inorganic perovskite materials spanning fundamental crystal chemistry, fabrication methodologies, device physics, stability mechanisms, optoelectronic applications, and future prospects in the context of their transformative potential for solar energy conversion and optoelectronic technologies. The central conclusion is that inorganic caesium lead halide perovskites represent a scientifically compelling and technologically promising class of materials, offering a unique combination of tunable optoelectronic properties, intrinsic thermal stability superior to hybrid organic–inorganic counterparts, and compatibility with both high-throughput solution processing and sophisticated nanoscale engineering. The past five years (2021–2026) have witnessed remarkable progress: PCEs in CsPbI₂Br and black-phase CsPbI₃ systems have surpassed 18–21% under optimized laboratory conditions; CsPbBr₃ nanocrystal LEDs have achieved EQEs exceeding 22% (Ling et al., 2023); photodetectors based on CsPbBr₃ single crystals have demonstrated world-class specific detectivities (Gao et al., 2016); and machine learning-guided materials discovery has begun to compress the experimental timescale for composition and process optimization from years to months. Simultaneously, the field has made significant strides in elucidating and mitigating the stability–efficiency trade-offs that have historically constrained inorganic perovskite device lifetimes, through advances in surface passivation, encapsulation, compositional engineering, and 2D–3D heterostructure design.

However, critical challenges persist. The thermodynamic instability of the photoactive CsPbI₃

black phase at room temperature remains unresolved, despite intensive research. Lead toxicity and the regulatory uncertainty surrounding its use impose increasingly urgent requirements for the development of high-efficiency lead-free alternatives a challenge for which current double perovskite and Sn-based compositions provide only partial solutions. Large-area manufacturing scalability, long-term operational stability certification, and end-of-life material recovery infrastructure require continued investment and innovation.

The field of inorganic perovskites stands at an inflection point where the cumulative weight of scientific understanding is sufficient to envision viable technological pathways to commercialization, but where the engineering and regulatory challenges of real-world deployment demand sustained, multidisciplinary effort. The integration of computational materials science, autonomous experimentation, device engineering, encapsulation technology, and environmental science will be required to navigate this complex landscape and realize the full potential of inorganic perovskites in a sustainable energy future. The coming decade promises to be transformative, and this review aims to provide a rigorous scientific foundation for the researchers and engineers who will drive that transformation.

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