Review

$Cs_2AgBiBr_6$ for Solar and Beyond: Technical Applications, Challenges, and Future Directions

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$Cs_2AgBiBr_6$ for Solar and Beyond: Technical Applications, Challenges, and Future Directions

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Abstract

The all-inorganic double perovskite $Cs_2AgBiBr_6$ has emerged as one of the most studied lead-free alternatives to conventional lead-halide perovskites, thanks to its outstanding chemical stability, pronounced defect tolerance, and negligible environmental toxicity. While its relatively wide indirect bandgap (approximately 1.95–2.2 eV) restricts the efficiency achievable in single-junction solar cells, this same characteristic proves advantageous for applications requiring high durability, extended carrier lifetimes, and low dark current — notably as the wide-gap component in tandem photovoltaic stacks, high-performance photodetectors, and ionizing radiation sensors. In recent years, researchers have also demonstrated the material's promise in low-dimensional forms such as colloidal nanosheets and nanocrystals, where quantum confinement effects enable modified electronic structure and enhanced optical response, paving the way toward potential uses in quantum photonics and confined charge-transport devices. Performance enhancement strategies documented in related studies include compositional tuning via halide or cation alloying, surface defect mitigation through various passivation approaches, nanoscale morphology control, and careful interface engineering. Important practical considerations — especially the relatively high cost of silver and challenges associated with large-scale synthesis — continue to influence the material's commercial prospects. The present review synthesizes the latest developments concerning pure $Cs_2AgBiBr_6$ and its derivative compositions, critically assesses its diverse technological roles spanning energy conversion, detection, and emerging quantum-related applications, and identifies promising research trajectories such as optimized tandem integration, scalable crystal growth methods, and machine-learning-assisted materials exploration. Drawing from relevant publications, this work offers a comprehensive, up-to-date outlook on the pathways through which $Cs_2AgBiBr_6$ may mature into a key material platform for next-generation sustainable optoelectronics and quantum technologies.

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Introduction

Halide perovskites have dramatically transformed the landscape of optoelectronic materials, particularly in the field of photovoltaics, owing to their outstanding charge transport properties, widely tunable bandgaps, and compatibility with low-cost, solution-based fabrication methods [1]. Lead-containing compositions such as methylammonium lead iodide ($MAPbI_3$) have achieved certified power conversion efficiencies exceeding 25% [2]; however, serious concerns regarding lead toxicity and poor long-term stability under moisture, oxygen, and illumination continue to pose major obstacles to large-scale commercial deployment [3].

These limitations have driven extensive global efforts to develop non-toxic, lead-free alternatives. Among the various families explored, halide double perovskites with the general formula $A_2B(I)B(II)X_6$ have emerged as particularly promising candidates due to their structural similarity to the classic ABX_3 perovskites combined with significantly improved chemical robustness and environmental safety [4,5].

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Within this class, the all-inorganic compound $Cs_2AgBiBr_6$ has received the greatest research attention. It crystallizes in a cubic double perovskite structure (space group $Fm^{-}3m$) featuring an ordered rock-salt arrangement of Ag^{+} and Bi^{3+} cations on the B-sites, which confers exceptional thermal, photochemical, and hydrolytic stability [1,6]. Although its indirect bandgap of approximately 1.95–2.2 eV represents a fundamental limitation for single-junction solar cells [7], this same wide bandgap is highly advantageous for use as the top absorber in multi-junction (tandem) architectures, as well as in radiation detectors and low-dark-current photodetectors [8,9].

Recent related literature has revealed the remarkable functional versatility of $Cs_2AgBiBr_6$ beyond conventional photovoltaics. Strategic compositional engineering — including partial halide exchange (Cl^{-}/Br^{-} or Br^{-}/I^{-}) and B-site cation alloying (Al^{3+}, Ga^{3+}, In^{3+}, Sb^{3+}, etc.) — has enabled controlled reduction of the bandgap and partial optimization of the optical transition, leading to markedly improved visible-light absorption [10,11]. Surface defect passivation using ionic liquids, organic ligands, polymers, or hydrogen treatments has significantly extended carrier lifetimes and enhanced device operational stability [12,13]. Most strikingly, the successful synthesis of colloidal quasi-2D nanosheets and nanocrystals has introduced strong quantum confinement effects, resulting in enhanced photoluminescence, modified electronic structure, and superior performance in photodetectors and emerging quantum-related applications [9,14,25].

The present review is motivated by three primary objectives:

1. To systematically consolidate and synthesize the rapidly expanding body of related experimental and theoretical studies on $Cs_2AgBiBr_6$ and its compositional derivatives.
2. To critically examine the most effective strategies for overcoming the material's principal intrinsic limitations, including its indirect bandgap and the economic challenges associated with silver.
3. To identify and prioritize the most promising future research directions capable of accelerating the transition of $Cs_2AgBiBr_6$ from promising laboratory material toward scalable, industrially relevant, sustainable technologies.

Historically, double perovskites were conceived as structural analogues of lead halide perovskites specifically designed to preserve desirable optoelectronic characteristics while completely eliminating lead-related toxicity [4]. Early structural and optical characterization of $Cs_2AgBiBr_6$ confirmed its cubic symmetry at room temperature and superior ambient stability compared with most Pb-based analogues [1]. This robustness has positioned $Cs_2AgBiBr_6$ as the current benchmark compound within the broader family of lead-free double perovskites, including Cs_2TiBr_6, $Cs_2AgInCl_6$, and Cs_2PtI_6, each exhibiting distinct bandgap and electronic characteristics but sharing the common advantage of defect-tolerant behavior [8].

Compared with other prominent lead-free candidates — such as tin-based (Cs_2SnI_6) or titanium-based (Cs_2TiBr_6) double perovskites — $Cs_2AgBiBr_6$ offers a particularly favorable combination of long-term chemical stability, shallow native defect states, and a wide bandgap ideally suited for tandem and detection applications [8,15]. Computational and experimental doping/alloying studies have repeatedly demonstrated viable pathways for bandgap reduction and enhanced optical absorption through controlled substitution at the Ag/Bi or halide sites [10,11].

Beyond energy harvesting, $Cs_2AgBiBr_6$ has shown strong potential in high-sensitivity photodetection and ionizing radiation sensing. Colloidal quasi-2D nanosheets exhibit significantly higher responsivity and faster response dynamics compared with bulk crystals, highlighting the critical role of dimensionality reduction in device performance [9]. Meanwhile, large single crystals have been successfully employed for gamma-ray and hard X-ray detection, taking advantage of their high resistivity, low leakage current, and excellent radiation hardness [16].

Perhaps most excitingly, the material is beginning to bridge the gap between conventional optoelectronics and emerging quantum technologies. Strong quantum confinement realized in nanosheets and nanocrystals enables substantial modification of the band structure, enhanced optical nonlinearity, and the possibility of single-photon emission or quantum light sources [9,14].

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The inclusion of a dedicated discussion on quantum-related applications within the technical applications section of this review reflects this rapidly expanding research frontier. By integrating recent experimental results with high-level computational insights this work aims to provide a balanced, up-to-date assessment of how $Cs_2AgBiBr_6$ may evolve from a robust lead-free photovoltaic candidate into a multifunctional platform for sustainable optoelectronics, radiation detection, and next-generation quantum technologies.

Crystal Structure and Fundamental Properties of $Cs_2AgBiBr_6$

1. Crystal Structure

$Cs_2AgBiBr_6$ adopts a cubic double perovskite structure at room temperature, belonging to the space group **$Fm^{-}3m$** (No. 225) [1,6]. The framework consists of a rock-salt ordered arrangement of Ag^+ and Bi^{3+} cations occupying the octahedral B-sites, resulting in alternating $[AgBr_6]^{5-}$ and $[BiBr_6]^{3-}$ octahedra that share corners to form a three-dimensional network. Cesium ions are located in the cuboctahedral A-sites, coordinated by twelve bromide anions [1].

High-resolution diffraction experiments have confirmed that the material remains cubic between approximately 120 K and 400 K [1]. Below ~120 K, a gradual transition to a tetragonal phase (space group **I4/m**) occurs due to the freezing of cooperative octahedral rotations and anisotropic bromide displacements along the Ag–Br–Bi axes [17]. Despite the larger ionic radius of Ag^+ compared with Bi^{3+}, the Ag–Br and Bi–Br bond lengths remain nearly identical (~2.81–2.82 Å), which is attributed to increased covalency in the $AgBr_6$ octahedra [1,6].

2. Electronic Band Structure

$Cs_2AgBiBr_6$ is an indirect bandgap semiconductor with a bandgap energy most commonly reported between **1.95 eV and 2.2 eV**, depending on measurement technique and sample quality [7,18]. The valence band maximum (VBM) is primarily composed of hybridized Ag 4d and Br 4p states with pronounced antibonding character, while the conduction band minimum (CBM) is dominated by Bi 6p orbitals with minor Br 4p contribution [10,15].

This orbital composition leads to relatively flat bands near both edges, which is the main origin of the indirect nature of the transition (typically $\Gamma \rightarrow X$ or similar points) and the correspondingly weak oscillator strength near the absorption onset [7]. First-principles calculations using hybrid functionals consistently reproduce this indirect character and highlight the material's exceptional defect tolerance: most native defects (vacancies, antisites, interstitials) form shallow rather than deep trap states due to the antibonding VBM pushing defect levels toward or into the bands [10,15].

3. Optical Properties

The optical absorption spectrum of $Cs_2AgBiBr_6$ reflects its indirect bandgap, showing a gradual onset with relatively low absorption coefficient immediately above the band edge [1,7]. Exciton binding energies are estimated in the range **100–300 meV**, substantially higher than in lead-based perovskites, which is attributed to reduced dielectric screening and stronger electron-hole Coulomb interaction [7,18,26].

Room-temperature photoluminescence is typically weak and broad, consistent with indirect transitions and efficient phonon-assisted recombination [1,7]. However, strong enhancement of emission efficiency and significant blueshift of the optical gap are observed in low-dimensional structures (quantum dots, nanosheets, nanoplatelets) due to quantum confinement effects [9,14,19].

4. Defect Chemistry and Stability

One of the most attractive features of $Cs_2AgBiBr_6$ is its pronounced defect tolerance. Unlike many conventional semiconductors, where vacancies and interstitials frequently create deep mid-gap states acting as efficient non-radiative recombination centers, the antibonding character of the VBM in this compound pushes most defect levels close to band edges or even resonant within the bands [10,15].

This shallow defect landscape, combined with the absence of toxic lead and the robust ionic framework, results in exceptional long-term stability under ambient conditions (moisture, oxygen, light) and elevated temperatures [1,12]. Carrier lifetimes in high-quality bulk crystals frequently exceed 1 μs (and can reach several microseconds with surface passivation), making the material

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particularly promising for applications requiring prolonged charge collection, such as radiation detectors and stable photovoltaic devices [9,16,26].

Technical Applications of $Cs_2AgBiBr_6$

The remarkable chemical robustness, long carrier lifetimes, high resistivity, and inherently low toxicity of $Cs_2AgBiBr_6$ have enabled its exploration across a remarkably broad range of optoelectronic and sensing technologies [5,9,19,26].

1. Solar Photovoltaics

The indirect bandgap of $Cs_2AgBiBr_6$ (≈1.95–2.2 eV) fundamentally limits the power conversion efficiency (PCE) achievable in single-junction devices, with most experimental values remaining below 5% [5,20]. However, this same wide bandgap is highly advantageous when the material is employed as the top subcell in tandem or multi-junction architectures, where it efficiently harvests high-energy photons while transmitting lower-energy light to narrow-gap bottom cells (silicon, Sn/Pb perovskites, etc.) [8,22,27].

Recent demonstrations have shown encouraging progress toward practical implementation. Blade-coated semi-transparent $Cs_2AgBiBr_6$ solar cells and small modules have achieved PCEs of ≈3.1% under standard 1-sun illumination and up to ≈7.7% under typical indoor lighting conditions, simultaneously exhibiting average visible transmittance (AVT) values exceeding 66%, promising light utilization efficiency (LUE), and acceptable color rendering index (CRI) — all critical metrics for building-integrated photovoltaics (BIPV) [23,24]. Targeted compositional modifications have further improved performance: partial gallium substitution ($Cs_2Ag_{0.95}Ga_{0.05}BiBr_6$) reduces the effective bandgap, increases open-circuit voltage and fill factor, and raises PCE from ≈3.5% to ≈4.5% [11,20]. Hydrogenation treatments have demonstrated even more substantial bandgap narrowing (down to ≈1.64 eV) while maintaining excellent stability, pushing single-junction PCE values toward 6.4% [3].

These results strongly support the continued development of $Cs_2AgBiBr_6$ for lead-free semi-transparent, indoor, and tandem photovoltaic systems.

2. Photodetectors

$Cs_2AgBiBr_6$ exhibits intrinsically low dark current, very high resistivity (>10^9 Ω·cm), and extended carrier lifetimes — properties that are highly desirable for high-sensitivity visible and near-UV photodetection [9,19].

The most significant recent advances have come from low-dimensional architectures. In 2025, colloidal quasi-2D $Cs_2AgBiBr_6$ nanosheets (lateral dimensions up to 1.4 μm, thickness a few nm) were synthesized via low-temperature methods and used to fabricate simple, transport-layer-free photodetectors. These devices achieved outstanding performance metrics: specific detectivity (D*) of 1.15 × 10^{12} Jones, responsivity (R) of 121 mA W^{-1}, on/off ratio exceeding 2.4 × 10^4, and fast rise/decay times of ≈857 μs / 829 μs. Crucially, the photodetectors retained full initial photocurrent after 80 days of storage under ambient conditions, demonstrating excellent operational stability [9,19].

Such results position quasi-2D $Cs_2AgBiBr_6$ nanosheets as one of the most promising lead-free materials platforms currently available for high-performance, stable, and potentially low-cost photodetectors.

3. Radiation Detection

The combination of high effective atomic number (heavy Bi and Ag atoms), ability to grow large, high-quality single crystals with low defect density, and very high resistivity makes $Cs_2AgBiBr_6$ particularly well-suited for X-ray and gamma-ray detection [10,16].

Single-crystal devices exhibit excellent linear response to low-energy X-rays, with mobility-lifetime products adequate for practical dosimetry and imaging applications [10,16]. Heterojunction architectures (e.g., $Cs_2AgBiBr_6/Cs_3Bi_2Br_9$) have delivered very high sensitivities — up to 1390 μC Gy^{-1} cm^{-2} at 100 keV and even higher at elevated temperatures — together with ultra-low detection limits and remarkable thermal stability [4]. Cation engineering (Eu^{3+} doping, organic cation substitution) has further enhanced X-ray sensitivity and photoconductive gain in bulk crystals [6].

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These characteristics establish $Cs_2AgBiBr_6$ as one of the leading lead-free candidates for next-generation radiation detectors in medical imaging, security inspection, nuclear safeguards, and environmental monitoring.

4. Emerging and Quantum-Related Applications

Beyond established photovoltaic and detection technologies, $Cs_2AgBiBr_6$ is showing early promise in several additional domains, including visible-light photocatalysis, room-temperature gas/ozone sensing, and high-mobility thin-film transistors [14,21].

Most significantly, strong quantum confinement realized in colloidal nanosheets and nanocrystals dramatically alters the electronic structure, greatly enhances photoluminescence quantum yield, and enables modified optical nonlinearity — opening realistic pathways toward single-photon sources, quantum light emitters, and nanoscale quantum-confined charge transport devices [9,14,19].

Collectively, the progress achieved between 2022 and 2025 — particularly in quasi-2D nanosheets, targeted compositional tuning, scalable semi-transparent modules, and heterojunction radiation detectors — clearly demonstrates that $Cs_2AgBiBr_6$ has evolved into a highly versatile, stable, and environmentally benign platform material capable of addressing diverse challenges across conventional and emerging optoelectronic technologies.

Methods for Improving the Properties of $Cs_2AgBiBr_6$

Despite its intrinsic advantages of exceptional stability and defect tolerance, $Cs_2AgBiBr_6$ suffers from several fundamental limitations — most notably its indirect and relatively wide bandgap, modest near-band-edge absorption coefficient, and residual surface recombination losses. A large body of recent research has focused on systematic strategies to mitigate these drawbacks and unlock higher device performance [5,10,20].

1. Bandgap Engineering

The indirect character and ~1.95–2.2 eV magnitude of the bandgap severely restrict single-junction photovoltaic efficiency. The most widely pursued approach involves compositional alloying at both the halide and B-cation sites.

Partial halide substitution ($Cl^- \rightarrow Br^-$ or $I^- \rightarrow Br^-$) allows fine-tuning of the bandgap and can partially optimize the optical transition by modifying orbital overlap and band dispersion [10,11]. Cation alloying at the Ag^+/Bi^{3+} sites — most notably with Ga^{3+}, In^{3+}, Al^{3+}, Sb^{3+}, or even controlled disordering of the Ag/Bi sublattice — has proven particularly effective. Gallium incorporation ($Cs_2Ag_{1-x}Ga_xBiBr_6$ with $x \approx 0.05$) has been shown to reduce the effective bandgap, enhance visible-light absorption, and deliver clear improvements in open-circuit voltage and overall power conversion efficiency [11,20]. Similar trends have been observed with aluminum and antimony doping, often guided by high-throughput DFT screening [10,11,20].

2. Defect Passivation and Surface Treatment

Although native defects in $Cs_2AgBiBr_6$ are predominantly shallow, surface halide vacancies (especially Br^-) and under-coordinated metal sites still contribute significantly to non-radiative recombination, particularly in thin films and nanostructures [10,15,20].

Effective passivation strategies include:

- treatment with ionic liquids or halide salts during film formation [12],
- organic ligand binding (e.g., fused-ring electron acceptors or phenylethylammonium halides),
- post-synthesis hydrogen or atomic-passivation treatments,
- and polymer encapsulation layers [3,13].

These approaches have been shown to dramatically extend carrier lifetimes (often from hundreds of ns to several μs), suppress trap-assisted recombination, and markedly improve device stability under continuous illumination and humidity stress [3,12,13].

3. Nanostructuring and Dimensional Reduction

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Reducing dimensionality to 0D (quantum dots), quasi-2D (nanosheets), or 1D (nanowires) forms introduces strong quantum confinement, which simultaneously blueshifts the bandgap, greatly enhances photoluminescence quantum yield, and modifies electronic band structure in ways beneficial for light emission and charge separation [9,14,19].

Colloidal synthesis routes have enabled the production of stable, solution-processable quasi-2D $Cs_2AgBiBr_6$ nanosheets with thicknesses of only a few unit cells. These structures exhibit significantly higher responsivity, faster response times, and much better ambient stability compared with their bulk counterparts when employed in photodetectors [9,19]. Nanostructuring is currently considered one of the most powerful tools for unlocking enhanced performance in detection, emission, and emerging quantum-confined applications [9,14].

4. Interface and Charge Transport Layer Engineering

Device performance is strongly governed by the quality of interfaces between the $Cs_2AgBiBr_6$ absorber and adjacent charge transport layers. Optimized electron transport layers (TiO_2, SnO_2, ZnO) and hole transport layers (NiO_x, Cu_2O, Spiro-OMeTAD alternatives) have been shown to reduce interfacial recombination, improve charge selectivity, and enhance extraction efficiency — particularly critical in tandem cell configurations [8,22,27,28].

5. Advanced Processing and Scalable Fabrication

The choice of synthesis route profoundly impacts film quality, defect density, and ultimately device reproducibility. While early studies relied on solution spin-coating, recent work has demonstrated scalable methods such as blade-coating, slot-die coating, and IR-assisted crystallization, enabling uniform large-area films with reduced defect concentrations and improved optoelectronic quality [23,24]. Ambient and green solvent processing routes further enhance environmental compatibility and industrial feasibility [7].

Taken together, these complementary strategies — bandgap engineering, surface passivation, dimensionality reduction, interface optimization, and scalable processing — have collectively driven steady performance gains across photovoltaic, photodetector, and radiation detection applications, while preserving the core advantages of stability and non-toxicity that make $Cs_2AgBiBr_6$ so attractive.

Environmental, Health, and Economic Considerations

While the elimination of lead is the most prominent advantage of $Cs_2AgBiBr_6$, a balanced evaluation of its broader environmental footprint, health implications, and economic feasibility is essential for realistic assessment of its long-term viability in commercial optoelectronic technologies [4,5].

1. Environmental Impact

The complete removal of lead represents the single greatest environmental benefit compared with conventional lead-halide perovskites. Lead is a persistent, bioaccumulative toxin; degradation or improper disposal of Pb-based devices can release soluble Pb^{2+} ions into soil and water, creating long-term ecological and human health risks [2,29].

By contrast, $Cs_2AgBiBr_6$ contains no lead, and both bismuth and silver exhibit considerably lower acute and chronic ecotoxicity under normal environmental conditions [4,5]. Nonetheless, silver mining and refining carry non-negligible environmental costs, including high energy consumption, water usage, potential acid mine drainage, and emissions of sulfur compounds or other heavy metals [2,6]. Bismuth is most often obtained as a by-product of lead, copper, or tungsten mining, which indirectly links its supply chain to other resource impacts.

Preliminary lifecycle assessment studies suggest that lead-free double perovskites like $Cs_2AgBiBr_6$ can achieve substantially lower overall ecotoxicity scores than Pb-based systems, provided silver usage is minimized through alloying and effective end-of-life recycling is implemented [6,18,26].

2. Health and Safety

From a direct human health perspective, $Cs_2AgBiBr_6$ is significantly safer than lead-containing perovskites. Chronic exposure to even low levels of lead can cause severe neurological,

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developmental, and cardiovascular damage [2]. Silver and bismuth compounds, while not entirely innocuous, have much lower toxicity profiles and are already used safely in medical (e.g., bismuth pharmaceuticals) and consumer applications (e.g., silver-containing antimicrobial coatings) under established regulatory guidelines [5].

During synthesis and device fabrication, standard chemical safety precautions are required when handling bromine-containing precursors (corrosive and irritant vapors). Appropriate engineering controls (fume hoods, ventilation) and personal protective equipment mitigate these risks effectively [7]. In finished, encapsulated devices, the risk of exposure during normal operation or accidental breakage is minimal [12,13].

3. Economic Feasibility

The primary economic challenge associated with $Cs_2AgBiBr_6$ is the substantially higher cost and more constrained global supply of silver compared with lead [2,8]. Silver prices are typically 50–100 times higher than lead per unit mass, and supply volatility can affect large-scale production economics [2,8].

Several mitigation strategies are actively being pursued in the literature:

- partial substitution of Ag^+ with lower-cost alkali (Na^+, K^+) or other cations while preserving structural integrity and optoelectronic quality [9,11],
- development of highly efficient, material-lean thin-film and nanostructured architectures to reduce the total amount of silver required per device [7,23,24],
- exploration of scalable, low-waste fabrication methods (blade-coating, slot-die coating, ambient/green processing) that improve material utilization and lower overall production costs [7,23,24].

Bismuth and cesium precursors are relatively inexpensive and abundant, which helps offset the silver cost burden.

4. Lifecycle and Sustainability Outlook

Early lifecycle analyses indicate that $Cs_2AgBiBr_6$-based devices can offer improved sustainability profiles compared with Pb-perovskites — particularly in terms of reduced hazardous waste generation, lower human/ecological toxicity potential, and higher recyclability of valuable elements (silver and bismuth) [6,18]. The material's superior long-term stability under real-world stressors (heat, humidity, light) further supports a favorable lifecycle outlook [1,5].

Responsible management of silver — through compositional reduction, improved recycling, and supply-chain transparency — will be critical to realizing the full sustainability advantages of $Cs_2AgBiBr_6$ over conventional lead-based technologies.

Significant Advances in Recent Research on $Cs_2AgBiBr_6$ and Its Derivatives

The period 2023–2025 has witnessed particularly rapid progress in the study of $Cs_2AgBiBr_6$, with publications documenting major breakthroughs in synthesis, dimensionality control, device performance, and functional diversification [5,9,19,20,23,24].

1. Experimental Breakthroughs in Synthesis and Nanostructuring

One of the most impactful recent developments has been the successful low-temperature colloidal synthesis of quasi-2D $Cs_2AgBiBr_6$ nanosheets with controlled lateral sizes (up to ≈1.4 μm) and few-unit-cell thicknesses [19]. These nanosheets exhibit strong quantum confinement, dramatically enhanced photoluminescence, and superior charge separation compared with bulk crystals. Transport-layer-free photodetectors fabricated from these nanosheets achieved record performance metrics for the material class, including specific detectivity of 1.15×10^{12} Jones, responsivity of 121 mA W^{-1}, and excellent 80-day ambient stability [19].

Concurrently, scalable ambient and green processing routes using ethyl acetate as both precursor solvent and antisolvent have produced high-quality, uniform thin films with reduced defect density, enabling semi-transparent solar cells and small modules with promising efficiency, visible transmittance, and color rendering characteristics [7,23,24]. Blade-coating has further

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advanced toward practical large-area fabrication, delivering reproducible semi-transparent photovoltaic modules suitable for building-integrated applications [23,24].

2. Compositional Engineering and Bandgap Reduction

Targeted cation substitution has delivered some of the most significant single-junction efficiency improvements reported to date. Partial gallium incorporation ($Cs_2Ag_{0.95}Ga_{0.05}BiBr_6$) reduces the effective bandgap, increases absorption coefficient, raises open-circuit voltage and fill factor, and boosts power conversion efficiency from ≈3.5% to ≈4.5% while maintaining excellent stability [11,20]. Similar trends have been observed with aluminum and antimony alloying, often guided by high-throughput DFT calculations that predict optimal compositions for direct-transition character and enhanced visible-light harvesting [10,11,20].

Hydrogenation treatments represent another major breakthrough, narrowing the bandgap to ≈1.64 eV while preserving long-term stability and pushing single-junction PCE values toward 6.4% — among the highest yet reported for pure or lightly modified $Cs_2AgBiBr_6$ [3].

3. Device Demonstrations and New Functionalities

Practical device demonstrations have matured considerably. Blade-coated semi-transparent $Cs_2AgBiBr_6$ modules have shown competitive performance under both 1-sun and indoor illumination conditions, with average visible transmittance exceeding 66% and light utilization efficiency suitable for building-integrated photovoltaics [22–24]. Heterojunction X-ray detectors ($Cs_2AgBiBr_6/Cs_3Bi_2Br_9$) have achieved sensitivities up to 1390 μC Gy^{-1} cm^{-2} (100 keV) and even higher at elevated temperatures, together with ultra-low detection limits and excellent thermal stability [4].

Beyond photovoltaics and radiation detection, dimensional reduction has enabled entirely new applications. Quasi-2D layered derivatives incorporating long-chain alkylammonium cations exhibit outstanding moisture resistance and have been successfully employed for high-selectivity, room-temperature gas and ozone sensing [12]. Porous single-crystal architectures and high-mobility thin-film transistors further expand the functional scope toward flexible electronics and advanced sensors [14,21].

4. Comparative and Computational Progress

Comparative studies have solidified $Cs_2AgBiBr_6$'s position as the current benchmark among lead-free double perovskites, outperforming Cs_2TiBr_6 and Cs_2PtI_6 in combined stability and defect tolerance, even if single-junction efficiency remains lower [8]. High-throughput computational screening, defect-level analysis, and strain-engineering studies continue to provide critical guidance for future alloy design and performance optimization [10,15].

Taken together, the literature of 2023–2025 clearly shows that $Cs_2AgBiBr_6$ has transitioned from a promising but limited laboratory material into a highly versatile, increasingly practical platform with demonstrated advances across synthesis scalability, device efficiency, stability, and application diversity.

Future Research Directions

Despite the impressive progress documented in recent literature, several fundamental and practical challenges must still be addressed to enable $Cs_2AgBiBr_6$ to transition from a highly promising laboratory material to a truly competitive, industrially scalable platform for sustainable optoelectronics [5,8,20,23,24].

1. Advanced Bandgap Engineering and Direct-Transition Pathways

The persistent indirect character of the bandgap remains the single most important intrinsic limitation for photovoltaic applications. Future efforts should focus intensively on deeper compositional space exploration — particularly multi-site alloying (simultaneous halide and B-cation substitution) and controlled Ag/Bi site disordering — with the explicit goal of achieving a pseudo-direct or fully direct bandgap while maintaining phase stability and defect tolerance [10,11,20].

High-throughput density functional theory combined with machine-learning accelerated screening will be essential to efficiently identify the most promising alloy compositions [15,16].

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Experimental validation of the most promising candidates should prioritize rapid, reproducible synthesis routes to close the prediction–realization loop as quickly as possible.

2. Multifunctional and Long-Term Defect Passivation

Although bulk defect tolerance is excellent, surface and grain-boundary traps continue to limit ultimate open-circuit voltages and carrier collection efficiencies, especially under prolonged operational stress.

Future research should target the development of multifunctional passivation strategies that simultaneously provide chemical protection, moisture/oxygen barrier properties, and optimized energetic alignment with transport layers [3,12,13,25]. Novel dopant-free hydrophobic polymers, self-assembled monolayers with dual binding motifs, and hybrid organic–inorganic encapsulation schemes are particularly promising directions.

Long-term operational stability testing (several thousand hours under combined heat, humidity, light, and electrical bias) on passivated devices will be critical to validate real-world durability.

3. Scalable Fabrication and Dimensional Control

Bridging the gap between small-area laboratory devices and large-area industrial modules remains a major challenge. Continued development of ambient, green, and high-throughput deposition methods (blade-coating, slot-die coating, spray-coating, roll-to-roll compatible processes) is essential [7,23,24].

Simultaneously, precise control over low-dimensional morphologies (quasi-2D nanosheets, quantum dots, nanowires) must be scaled while preserving colloidal stability, phase purity, and optoelectronic quality — a prerequisite for exploiting quantum confinement benefits in commercial photodetectors, light emitters, and quantum-related devices [9,14,19].

4. Tandem and Multi-Junction Integration

$Cs_2AgBiBr_6$'s wide bandgap makes it one of the most promising lead-free candidates for the top subcell in all-perovskite or perovskite-on-silicon tandems.

Future work should prioritize:

- development of transparent, low-resistance interconnect layers compatible with $Cs_2AgBiBr_6$,
- detailed interface studies to minimize recombination at the wide-gap/narrow-gap junction,
- and full device stability testing under realistic outdoor conditions [8,22].

Demonstration of stable tandem modules with total efficiencies significantly above 20% would represent a major milestone for lead-free perovskite photovoltaics.

5. AI/ML-Driven Materials Discovery and Optimization

Machine learning and artificial intelligence are rapidly emerging as powerful accelerators for perovskite research.

Future efforts should leverage AI-guided high-throughput screening of dopants, alloy compositions, surface ligands, and processing parameters, coupled with autonomous or semi-autonomous experimental validation loops [15,16].

Such approaches have the potential to dramatically shorten the time from new composition identification to functional device demonstration.

6. Diversification into Quantum and Radiation-Hard Technologies

The strong quantum confinement effects already demonstrated in quasi-2D nanosheets and nanocrystals open realistic pathways toward quantum photonics (single-photon sources, entangled photon pairs) and radiation-hard electronics [9,14,19].

Systematic investigation of confinement-tunable optical nonlinearities, spin–orbit coupling, and carrier dynamics in these low-dimensional systems should be prioritized.

Likewise, further optimization of single-crystal growth, heterojunction design, and doping strategies for X-ray/gamma detectors could position $Cs_2AgBiBr_6$ as the leading non-toxic material for next-generation medical imaging and security systems [4,6,10].

Addressing these interconnected directions — guided by the most recent open-access experimental and computational advances — will be decisive for determining whether $Cs_2AgBiBr_6$

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can fulfill its potential as a cornerstone material for sustainable, stable, and multifunctional optoelectronic technologies in the coming decade.

Conclusions

The all-inorganic double perovskite $Cs_2AgBiBr_6$ has clearly established itself as one of the most robust, versatile, and thoroughly investigated lead-free alternatives within the halide perovskite family [1,5].

Its cubic crystal structure, outstanding chemical and thermal stability, pronounced defect tolerance, long carrier lifetimes, and complete absence of toxic lead provide a strong foundation for a wide spectrum of applications — ranging from tandem and semi-transparent photovoltaics, to high-sensitivity photodetectors, ionizing radiation detectors, and emerging quantum-confined optoelectronic devices [5,9,19,23–25].

While the indirect bandgap of ≈1.95–2.2 eV continues to constrain single-junction photovoltaic efficiencies (most reported values still remain below 5%), recent open-access advances have demonstrated multiple viable pathways toward improved performance:

- targeted cation alloying (especially Ga^{3+} and Al^{3+} substitution) and hydrogenation have enabled significant bandgap reduction and higher single-junction PCEs (up to ≈6.4%) [3,11,20],
- colloidal quasi-2D nanosheets have delivered record photodetector metrics ($D^* \approx 1.15 \times 10^{12}$ Jones, excellent ambient stability) [9,19],
- scalable blade-coating and green processing have produced semi-transparent modules with promising efficiency, transmittance, and color quality suitable for building-integrated photovoltaics [23,24],
- heterojunction architectures have pushed X-ray detector sensitivities into the 1390–2075 $\mu C\ Gy^{-1}\ cm^{-2}$ range with ultra-low detection limits and impressive thermal resilience [4,6].

These collective achievements — all documented in publications between 2022 and 2025 — clearly illustrate that $Cs_2AgBiBr_6$ is no longer merely a conceptually interesting lead-free candidate, but rather a rapidly maturing multifunctional material platform.

At the same time, important challenges remain. The relatively high cost and supply constraints of silver continue to represent the dominant economic barrier to large-scale deployment [8]. Residual surface recombination, interfacial losses, and the need for more systematic long-term operational stability data under combined real-world stressors still require further attention [12,13].

Nevertheless, the outlook is distinctly positive. Ongoing research directions — particularly deeper compositional space exploration, multifunctional passivation schemes, scalable green fabrication, AI/ML-accelerated materials discovery, and targeted development of tandem cells and quantum-confined architectures — offer realistic pathways toward overcoming these remaining limitations [10,15,19,23,24].

When combined with responsible silver management (through alloying, reduced material usage, and effective recycling), $Cs_2AgBiBr_6$ holds strong potential to become a cornerstone material in the future landscape of sustainable, stable, non-toxic optoelectronics — capable of simultaneously addressing energy conversion, high-performance detection, and emerging quantum-related technologies.

By synthesizing the most recent open-access experimental results, computational insights, and device demonstrations, this review provides a comprehensive, up-to-date roadmap of both the achievements already realized and the critical next steps required to fully realize the transformative promise of $Cs_2AgBiBr_6$.

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