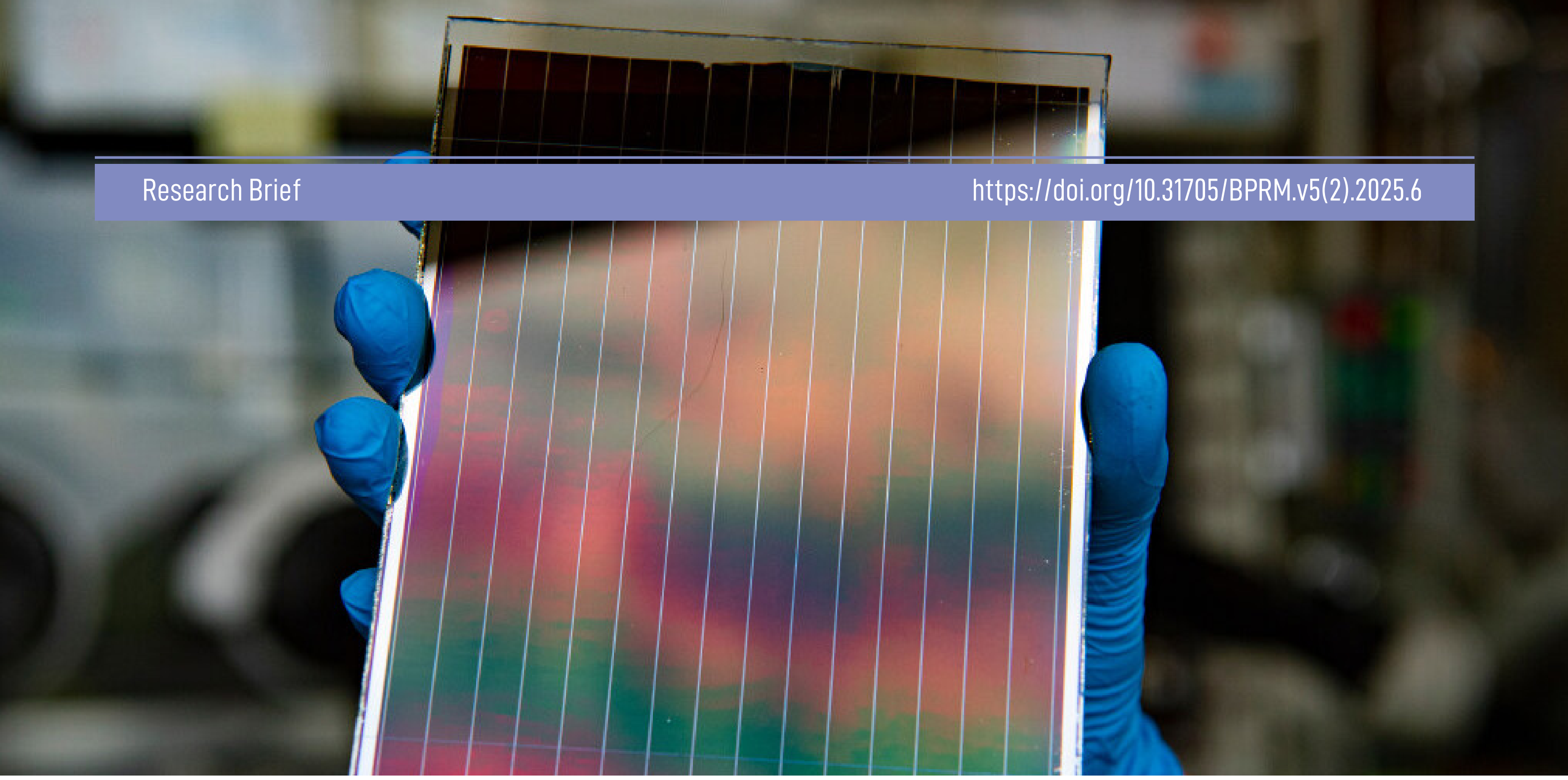

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Mitigation of Challenges in the Commercialization Pathway of Perovskite Solar Cells

In recent years, perovskite solar cells (PSC) have attracted significant interest in the solar cell industry due to their steep increase in photovoltaic performances, from 4% in 2009 to 26.7 % in 2025. The significant progress can be attributed to the outstanding optoelectronic properties of the perovskite materials, including low exciton binding energy at room temperature, strong light absorption, high carrier mobility, and tunable band gaps through compositional engineering. In addition, PSCs offer simple and affordable fabrication processes, making them an attractive alternative to silicon solar cells. The conventional 3D perovskite structure is denoted by the standard formula of ABX3, where A, B, X are a monovalent cation, a divalent metal cation, and a halide anion, respectively, as shown in Figure 1. Despite their advantages, PSC commercialization is hindered by stability and Pb-toxicity. Exposure of PSCs to heat, humidity, and UV light accelerates degradation, while Pb poses serious environmental and health risks due to potential leaching.

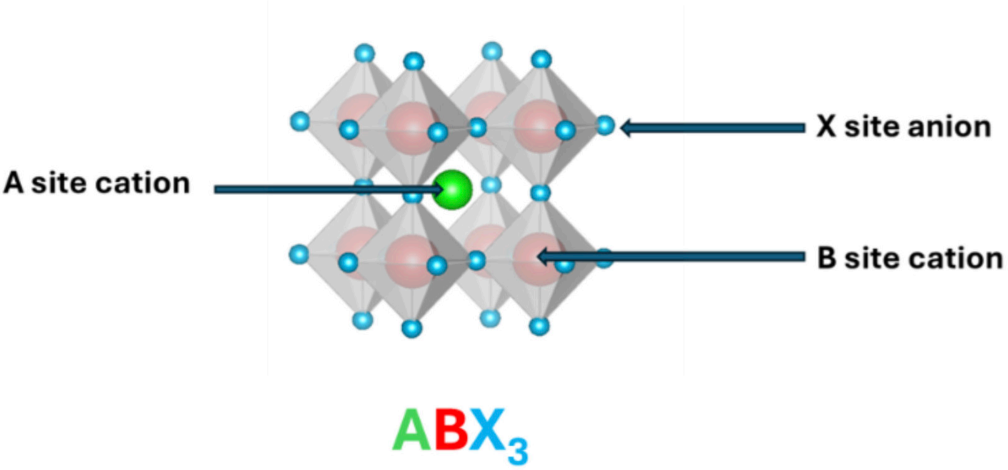

Figure 1. The structure of perovskite materials

Stability Challenges and Enhancement Strategies

The stability of PSCs is affected by the complex interplay of internal and external factors. The internal factors are interface defects and ion migration, both of which can accelerate carrier recombination and ion accumulation, ultimately reducing device performance and stability. Interface defects can be reduced through interface engineering and careful material selection. Compositional engineering of the perovskite layer and incorporation of additives suppresses the ion migration. External factors such as moisture, oxygen, UV radiation, elevated temperature, and other environmental conditions further exacerbate degradation, as shown in Figure 2. To overcome the chemical degradation reactions caused by moisture and oxygen, encapsulation strategies such as hydrophobic coatings and waterproof barrier films are employed to block the moisture ingress [2]. UV stabilization additives and protective coatings have been investigated to alleviate the UV light induced photochemical degradation. Furthermore, the thermal stability of PSCs is enhanced through compositional modification of the perovskite materials and charge transport layers to prevent phase transitions, suppress ion migration, and minimize other detrimental processes.

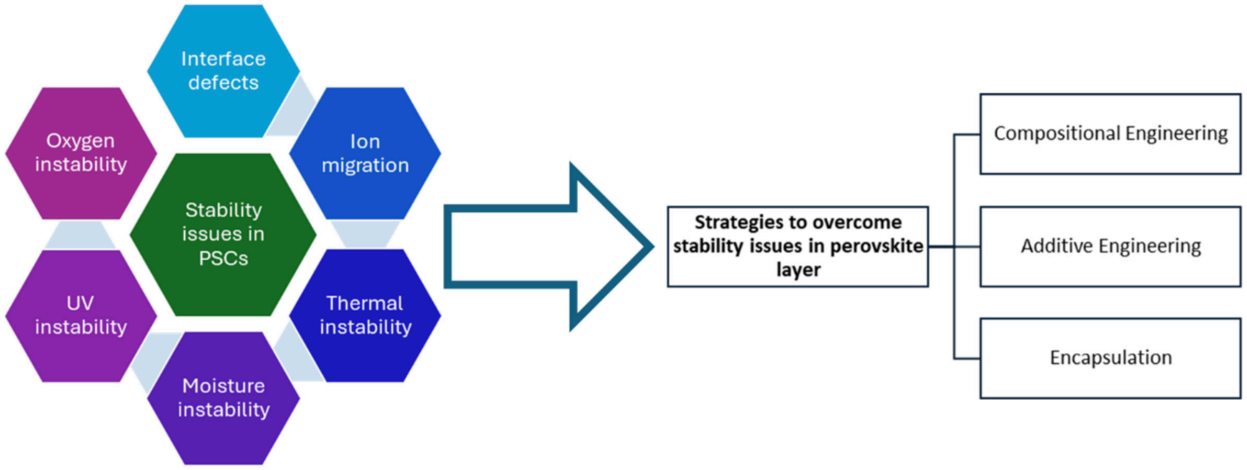

Figure 2. The stability issues faced by PSCs and stability enhancement strategies

Moreover, dimensional engineering of the PSCs has gained significant attention recently, due to remarkable improvements in stability, which involves modification of the conventional ABX3 three-dimensional lattice structure by incorporating alternative bulky A-site cations that promote the formation of 2D (layered) structures. 2D perovskite materials are represented by (RNH3)2(A)n-1BnX3n+1, where R is a large organic cation which functions as a spacer cation between the inorganic perovskite layers, creating a layered structure containing alternative organic and inorganic components. This layered configuration facilitates the separation of the inorganic layers, contributing to the development of a 2D structural framework. The enhanced stability of the 2D perovskites can be credited to their unique molecular arrangement featuring strong Hydrogen bonds between organic cations and inorganic octahedral layers, and the hydrophobic nature of the organic layers. Since the efficiency of 2D perovskite materials is relatively poor, 2D/3D mixed-dimensional perovskite materials have been developed, which offer a balance of efficiency and long-term operational stability. In our study, we numerically investigated a 2D/3D PSC using a 1.4-butanediamin spacer molecule-based 2D capping layer, achieving a PCE of 26.56%, and indicating a potential candidate for stability enhancement [3]. Despite these efforts, the stability of the PSCs is yet to be significantly improved to achieve the stability protocols established by the International Summit on Organic Photovoltaic Stability (ISOS) for commercialization. Looking ahead, all stability enhancement strategies including compositional engineering, interfacial passivation, dimensional tailoring, and advanced encapsulation, should be systematically optimized without undermining the low-cost benefit of PSCs to unlock long-term operational stability and enable the successful commercialization of perovskite solar cells.

Toxicity Challenges and Mitigation

The lead induced toxicity in PSCs is another critical commercialization barrier. Lead is a well-known neurotoxin, and its presence in PSCs raises serious environmental and health concerns, especially due to its high solubility in water and tendency to leach as Pb^{2+} ions when the perovskite structure degrades under moisture, heat, or UV exposure. Studies have proven that even a single square meter of a PSC module can release up to 0.9 g/m2 of PbI$_2$ after rainfall, resulting a significant contamination risk unless properly diluted [4]. Different elements have been suggested as potential replacements for Pb^{2+} in the ABX$_3$ perovskite lattice, including tin (Sn^{2+}), germanium (Ge^{2+}), bismuth (Bi^{3+}), and antimony (Sb^{3+}), along with complex materials like chalcogenide and chalcohalide. Among these alternatives, tin-based perovskites such as MASnI$_3$ and FASnI$_3$ show comparable band gaps and charge transport properties to Pb based perovskite materials [5].

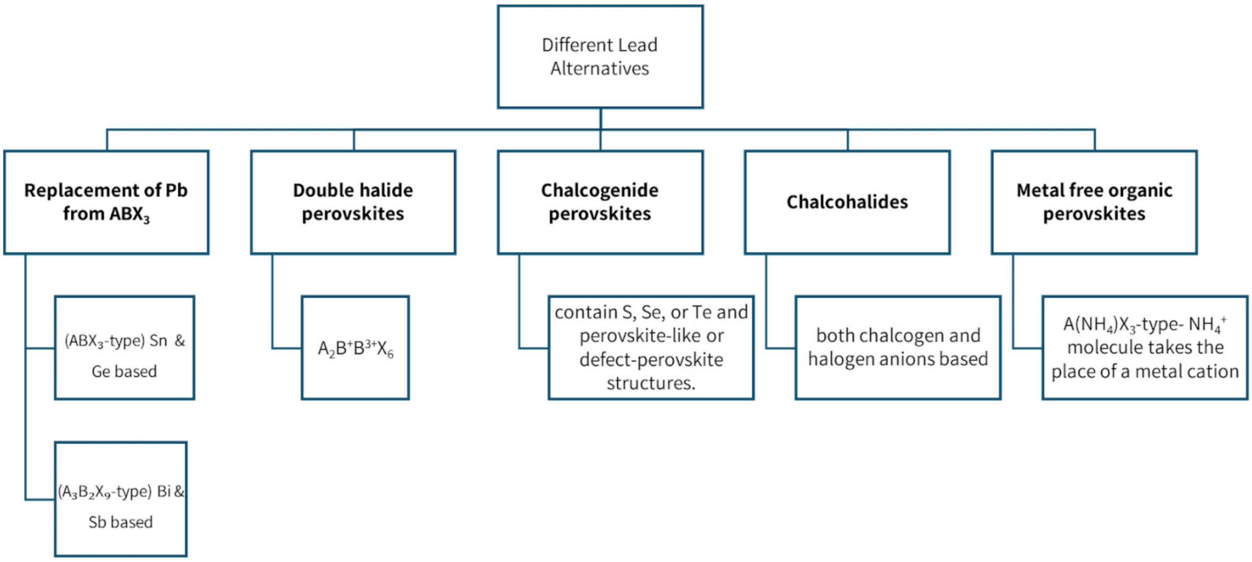

Figure 3. Potential alternative materials to Lead

However, Sn^{2+} based perovskites suffer from poor stability, as Sn2+ readily oxidize into Sn^{4+}. This oxidation leads to severe material degradation and high background carrier concentrations, resulting in deterioration of device performance. Germanium-based perovskites experience similar stability challenges, and their applications in PSCs are further limited by large band gaps and low efficiencies, which remain below 5%. Bismuth- and antimony-based compounds demonstrate enhanced chemical stability and reduced toxicity, and they form low-dimensional perovskite-like structures such as Cs$_3$Bi$_2$I$_9$ and Cs$_2$AgBiBr$_6$. Although their environmental advantages are as nontoxic materials, these materials typically show indirect band gaps, limited transport, and low light absorption, resulting in lower efficiencies, which are mostly below 5%.Chalcogenide perovskites, such as BaZrS$_3$, are considered completely lead-free materials which offer excellent thermal and chemical stability. However, they have indirect band gaps, high synthesis temperatures and poor photovoltaic performance. Chalcohalides are a class of chalcogenides which contain both chalcogen and halide anions. They are an emerging research area enabling better bandgap tunability and environmental resilience; however, they are still in an early development stage. Even though there are numerous research efforts towards lead alternatives, no lead-free perovskite material has yet aligned with the PCE conventional lead-based PSCs. The existing alternatives demonstrate PCE below 15% and lack the stability required for commercial application. These limitations highlight a critical research need to investigate and engineer new materials that balance high efficiency, long-term stability, and environmental and human safety. Future research directions focus on defect control, targeted interface engineering of the above-mentioned systems and compositional engineering of multi-element systems, such as Sn–Ge or Bi–Sb alloys, to enhance charge dynamics and structural resilience, and employing machine learning and high-throughput screening to accelerate the discovery of new candidate materials.

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