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Sustainable Energy Solutions: Enhancing the Efficacy and Stability of Lead Iodide Perovskite Solar Cells

Bangshidhar Goswami*

Abstract

Lead iodide perovskite solar cells have emerged as a transformative technology in the field of photovoltaics, demonstrating remarkable power conversion efficiencies that rival traditional silicon-based solar cells. However, concerns regarding their long-term stability and environmental impact pose significant challenges for their widespread adoption. This study investigates the current advancements in lead iodide perovskite solar cells, emphasizing strategies to enhance both their efficiency and stability. We explore innovative approaches, such as compositional engineering, interface modification, and encapsulation techniques that mitigate degradation mechanisms and extend operational lifetimes. Furthermore, the environmental implications of lead use in these solar cells are critically examined, proposing potential alternatives and recycling strategies to minimize ecological footprints. Our findings contribute to the ongoing discourse on sustainable energy solutions, highlighting the promise of lead iodide perovskite solar cells while addressing the crucial issues of stability and environmental safety. Scientists have been searching for a non-conventional, easily accessible, and sustainable energy source that primarily uses solar cells for a long time. Solar cells are a low-cost, carbon-emission-free energy source that converts light energy, or photons, directly into electrical current, or electrical energy, by utilizing the photovoltaic phenomenon. Perovskites, especially organic-inorganic halide perovskites, have become more and more popular recently because of their exceptional optical properties and low processing temperature requirements. The first developed perovskite solar cell was introduced in 2009 when $CH_3NH_3PbI_3$ organometallic perovskite with a liquid-based hole transport layer was added to a dye-sensitized solar cell.

Keywords: Perovskite solar cells, efficiency, stability, environmental impact, compositional engineering

INTRODUCTION

The lead iodide Perovskite Solar Cell (PSC) has garnered the interest of researchers recently due to its exceptional potential to surpass conventional silicon solar cells. Research on PSCs has primarily focused on lead iodide perovskites because of their incredibly high light-absorbing capacity. The Power Conversion Efficiency (PCE) of the initial PSC, which was created in 2009, was merely 3.8%. Ten years passed before the PCE rose to 25.2%. Even with their high PCE, they are still unsuitable for commercial use due to their short life. This article discusses the design of PSC devices, how to achieve higher PCE with specific configurations, and the stability problem with PSCs that keeps them from being used in commercial settings.

***Author for Correspondence**
Bangshidhar Goswami
E-mail: goswami.b8757@gmail.com

Former Assistant Professor, Metallurgical Engineering, RVS College of Engineering and Technology, Jamshedpur, Jharkhand, India.

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This resulted in only 3.8% of the total PCE. In 2012, the first solid-state type PSC was introduced,

boasting a 9.7% PCE. This was made possible by using spiro-OMeTAD as the hole transport layer in place of the liquid electrolyte. 2019 currently has the highest PCE of 25.2% for solar cells made from perovskites. PECs have superior PCE, but their lifetime is still not as long as that of silicon solar cells [1]. This is because variations in temperature, humidity, moisture content, and UV light can cause perovskites to become unstable. This instability is also exacerbated by the presence of lead (Pb), a poisonous substance that can have detrimental effects on health. Researchers are working around the clock to develop solutions for these issues to produce more practical, cost-effective, high-quality, and efficient PSCs.

Photonic Power Conversion Efficacy

The presence of excess lead iodide in halide perovskites (HaPs) has been linked to the achievement of a photon-to-PCE higher than 20%. To achieve even higher PCEs, it is imperative to understand the role of residual lead iodide in these perovskites. By assessing the impact of excess lead iodide in the perovskite film on the characteristics of film formation from grazing-incidence wide-angle X-ray scattering (GIWAXS) and high-resolution transmission electron microscopy (HR-TEM), as well as on charge diffusion length using electron-beam-induced current (EBIC) measurements, the suggestive issue investigated the mechanism enabling this effect. According to our research, an excess of lead iodide in the perovskite precursors may reduce the concentration of halide vacancies, which will lead to the formation of cubic α-perovskite crystals with azimuthal angles ranging from 0° to 90°. According to the descriptive issue, the nanostructured titanium dioxide layer contained more perovskite carriers than the capping layer. These results demonstrate the role of lead iodide and are in line with lead iodide-rich PSCs' enhanced performance [2]. Halide PSCs with organic cations have already achieved PCEs of more than 22% in a comparatively short amount of time. The main strategy for raising PSCs' PCEs has been to develop methods for depositing incredibly dense and homogeneous layers on substrates and controlling the ABX_3 composition of HaP, where X is halide. The composition of HaP materials can be controlled by varying the ratio of lead iodide (PbI_2) to the salt of the A cation, which is used to form the perovskite layers and can be either formamidinium iodide (FAI) or methylammonium iodide (MAI). The descriptive results show that adding excess PbI_2 to a solution used to prepare a HaP of 15% methylammonium lead bromide ($MAPbBr_3$) mixed with 85% formamidinium lead iodide ($FAPbI_3$) significantly improves the PCEs of PSCs. The foundation of this HaP is $(FAPbI_3)_{0.85}(MAPbBr_3)_{0.15}$). However, it is unclear how much of the efficiency gain in these PSCs comes from residual PbI_2 in the HaP layer and excess PbI_2 in the precursor solution (which is made by adding PbI_2 above the required (MAX or FAX) to PbI_2 ratio). It is still unknown where the remaining PbI_2 is in the HaP and how it is currently being used. While several previous studies have looked at the effect of excess PbI_2 in HaPs, the details of this phenomenon could not be explained, and the theories proposed to explain these effects are not comprehensive. PbI_2, for example, has been suggested to be present at the interfaces between nanostructured titanium dioxide (ns-TiO_2) and HaPs, as well as at the grain boundaries and HaP film surface. Descriptive issued grazing-incidence x-ray scattering (GIXS) was employed to obtain additional insights into the formation of distinct crystal orientations of HaPs ($CH_3NH_3PbI_3$) using various HaPs deposition techniques, including the commonly used one/two-step coating. The process of converting PbI_2 single crystal to $CH_3NH_3PbI_3$ was explained within the framework of structural relations and transformation dynamics. It was found that while the reaction initially proceeded topotactically, the memory of the initial PbI_2 morphology was eventually lost due to a destruction/reconstruction process.

Photoluminescence (PL) spectroscopy and time-correlated single photon counting (TCSPC) have been widely used to understand charge collection efficiencies and identify charge transfer mechanisms. However, exact values of electron/hole pair diffusion lengths in the actual PSCs for HaP materials have proven difficult to determine, because a model for the charge-quenching processes in different HaP layers needs to be developed. Additionally, it is crucial to verify that these techniques are applicable to mixed composition HaP layers. The descriptive issue examined key elements of the electrical and crystal properties of HaP layers with and without excess PbI2 using HR-TEM,

GIWAXS, and EBIC measurements. Our EBIC results show that excess PbI_2 reduces electronic defects in the bulk film, and GIWAXS indicates that the PbI_2-rich HaP film is textured and has more ordered grains than the normal film. Furthermore, HR-TEM observations show that excess PbI_2 surrounds the perovskite grains rather than just occurring at grain boundaries. These properties may improve charge transfer and lead to a PV cell with incredibly low hysteresis when compared to films and cells made from a stoichiometric solution precursor.

Flexible and Cost Efficacy

Flexible PSCs hold great potential for low-cost roll-to-roll production of thin single- and multijunction photovoltaic devices. Among the different deposition techniques used for the perovskite absorber, the two-step hybrid vacuum-solution approach allows for precise control of PbI_2 thickness and morphology. Nevertheless, the effective conversion to perovskite is limited by the organic cations' diffusion within the compact lead halide layer. This is a multistage absorber deposition made of thermally evaporating PbI_2 and spin-coating CH_3NH_3I (methyl-ammonium iodide).

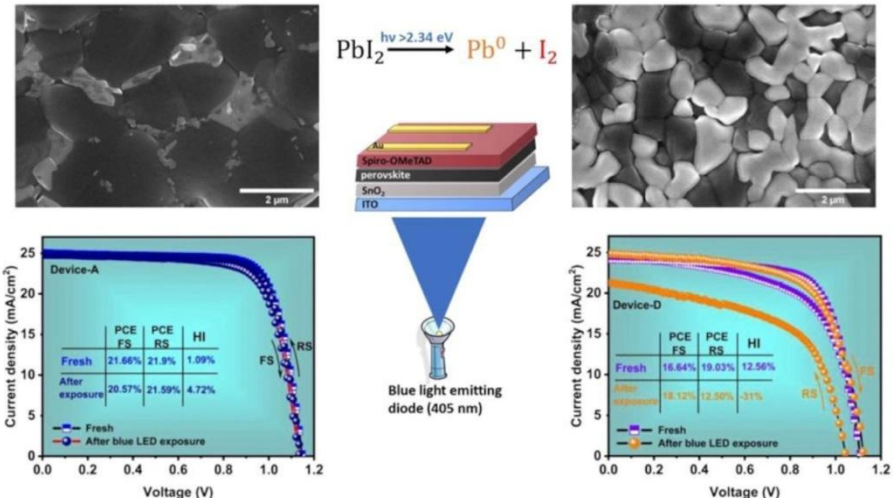

Figure 1. Researchers focus on the presence of residual PbI_2

The process is based on the different ways that PbI_2 is grown on crystalline and amorphous surfaces by vacuum deposition. This approach provides a way to effectively increase the absorber thickness while addressing the limited MAI diffusion in the compact PbI2 film through a two-step deposition process. Flexible PSC efficiency rises from 14.2 to 15.8% with multistage deposition. Furthermore, the use of the amorphous transparent conductive oxide (TCO), InZnO, improves the mechanical resistance against bending in comparison to conventional crystalline TCO-based flexible devices. In the development of near-infrared transparent flexible PSCs, an efficiency of 14.0% and an average transmittance of roughly 74% between 800 and 1000 nm are attained. Flexible perovskite/CIGS thin-film tandem devices with an efficiency of 19.6% are demonstrated in the four-terminal configuration [3]. Cost savings are possible because flexible photovoltaic devices can be produced using high throughput roll-to-roll manufacturing instead of traditional sheet-to-sheet methods. Hybrid organic-inorganic perovskites are a relatively new class of low-cost photovoltaic materials that have been developed recently. Perovskites are ideal absorbers for single- and multijunction devices due to their high absorption coefficient, low Urbach energy, and high bandgap (~1.6 eV). Among different perovskite-based multijunction technologies, all-thin-film perovskite/Cu(In,Ga)Se_2 (CIGS) tandem devices have shown an extraordinary performance improvement over the last three years, reaching efficiencies as high as 23.9% (Figure 1).

It should be noted that the top and bottom cells of these tandem devices are grown on rigid glass substrates. Flexible thin-film tandem devices have been made possible by the demonstration of highly efficient flexible perovskite and CIGS solar cells, which could lead to the roll-to-roll production of

lightweight perovskite-based multijunction devices in the future. A fascinating feature of PSCs is the high degree of flexibility offered by low-temperature deposition methods. One of the most promising deposition methods is the hybrid vacuum-solution two-step method, which produces compact absorber layers devoid of pinholes by precisely controlling the thickness and morphology of PbI_2. Conventional solution-based procedures, such as one- or two-step deposition require the use of dimethylformamide (DMF) and dimethyl sulfoxide (DMSO). These solvents should not be used with low-temperature, effective organic-based Electron Transport Layers (ETLs), such as C60. Nevertheless, the CH_3NH_3I (MAI) spin coating from isopropanol solution and the thermal evaporation of PbI_2 have no effect on the extremely thin organic charge extraction layer. Diffusion and intercalation of organic cations into the inorganic PbI_2 layered structure determines their conversion into high-quality perovskite absorbers in a two-step deposition process. As soon as the organic cation is deposited, the intercalation process starts at the edge-air interface, where organic moieties instantly form hydrogen bonds with the inorganic sites. Because there are no Van der Waals gaps in the perovskite structure, the abrupt formation of a thin layer of $CH_3NH_3PbI_3$ stops MAI cations from diffusing further to the inner lead sites. As a result, a carefully designed PbI_2 morphology is necessary to encourage MAI cation diffusion and is crucial for the transformation into a perovskite absorber. There are numerous documented techniques for effectively modifying PbI_2's morphology, which encourages the intercalation of organic cations. In the descriptive, it is possible to enhance the conversion to the perovskite phase by postponing PbI_2 compact-layer crystallization by coordinating with DMSO molecules. A detailed description of the solvent substitution method was given to control the growth and recrystallization of PbI_2 nuclei with precision. By using a mixed PbI_2: MAI precursor to pre-expand the PbI_2 layer, respect enhanced organic cation intercalation and conversion reaction. While these techniques are effective in increasing device efficiency, they are not applicable in the case of PbI_2 grown by vacuum deposition techniques. The growth of thermally evaporated PbI_2, which is created by a hybrid two-step vacuum-solution process, is influenced by the substrate surface. Thermal evaporation of PbI_2 onto amorphous surfaces results in a compact morphology and preferential growth parallel to the substrate due to the minimization of the combined surface and interface energy. On the other hand, anisotropic substrates and interface energy work together to produce a morphology onto crystalline substrates that resembles a nanoplate. To effectively increase the absorber thickness for the descriptive issue, a two-step hybrid vacuum-solution deposition method was modified. A multistage deposition process is used to customize the morphology of PbI_2. The first stage is characterized by a compact inorganic layer, while the second stage is characterized by a nanoplate-like morphology. By carefully screening the organic cation concentration and nanoplate-like PbI_2 thickness, we can demonstrate flexible PSC with a steady-state efficiency of 15.8%, in contrast to a 14.2% efficient device made using a conventional two-step hybrid process. For the TCO, the descriptive issue sputtered InZnO (IZO), which has a high near-infrared transparency and an amorphous nature. Extremely flexible PSCs can be obtained by comparing the latter properties with conventional flexible PSCs based on crystalline TCO. After 1000 bending cycles, the devices retain 90% and 80% of their initial efficiency at bending radii of 6 and 4 mm, respectively. Furthermore, the TCO can be used in tandem applications due to its high near-infrared transparency. Descriptive data were released on a NIR-transparent flexible PSC with a steady state efficiency of 14.0% and an average transmittance of about 74% between 800 and 1000 nm. By combining a flexible perovskite top cell with a flexible CIGS bottom cell, we demonstrate 19.6% efficiency in the four-terminal tandem configuration.

Stability and Low Toxicity

PSCs are a more competitive and attractive alternative. Unfortunately, their potential and future commercialization are limited by their relatively low stability and the toxicity caused by the lead content. Then, it appears that a crucial development axis is reducing lead content while increasing stability. According to recent reports, a new family of perovskite has been discovered that displays PbI+ unit vacancies inside the lattice. This is caused by the insertion of large organic cations that do not follow the Goldschmidt tolerance factor, such as hydroxyethylammonium ($HO\text{-}(CH_2)_2\text{-}NH^{3+}$ or

(HEA^+) and thioethylammonium ($HS\text{-}(CH_2)_2\text{-}NH^{3+}$ or (TEA^+). The lead-iodide-deficient Methylammonium lead triiodide ($MAPbI_3$) or Formamidinium lead triiodide ($FAPbI_3$) or (FAPI) network can integrate these perovskites. For lead and halide-deficient perovskites, they are known as d-HPs. They present a 3D shared $Pb_{1-x}I_{3-x}$ perovskite corner network. Innovative problem-solving solar cells by chemically engineering both systems. d-$MAPbI_3$ -HEA had a PCE of 11.47%, better stability, and 13% less lead than $MAPbI_3$. On the other hand, d-$FAPbI_3$ -TEA achieved a PCE of 8.33%, outperforming conventional α-FAPI in terms of perovskite film stability. The presence of TEA^+ within the lattice slows down the aging process of d-$FAPbI_3$ -TEA perovskite significantly by preventing α-FAPI degradation into yellow δ-$FAPbI_3$ through direct degradation into inactive Pb(OH)I. For hybrid HaPs, or PVKs, the general formula is ABX3. The formula Cs^+, CH_3NH_3 + (methylammonium, noted MA^+), or $HC(NH_2)_2$ + (formamidinium, noted FA^+) are examples of monovalent organic or inorganic cations. B is an octahedrally coordinated divalent metal ion (usually Pb^{2+} or Sn^{2+}), and X is a halogen (usually Cl^-, Br^-, or I). These substances crystallize into tetragonal or cubic shapes at room temperature. PVKs have attracted a lot of interest from the scientific community worldwide for a variety of optoelectronic applications, such as lasers, LEDs, photodetectors, scintillation, photocatalysis, and photovoltaic PSCs. After being introduced in 2009, PSCs have demonstrated great promise as materials for photovoltaic devices. Since then, a great deal of research has been conducted on PSCs because of their optoelectronic properties, which include long carrier diffusion lengths, low recombination loss, high absorption coefficients, high charge carrier mobility, and tunable bandgaps. Their PCE grew quickly as a result, and in 2022 it achieved a certified record efficiency of 25.7%. One of the most studied is perovskite methylammonium lead iodide, or $MAPbI_3$ (MAPI). However, the relatively low stability and toxicity of HaPs due to lead pose a challenge to their potential and eventual commercialization [4]. To solve the first problem and convert the reference $MAPbI_3$ perovskite into $MAPb_{1-x}AxX_3$, many studies have been carried out to partially or completely replace lead with less/non-toxic elements, such as Sn, Sr, Cu, Ag, or Ge. Except for Sn substitution, which can reach a high percentage level (up to 50% or more) and still reach high efficiency, other elements can only be added in very small amounts (less than 5%), which is insufficient. Research on encapsulation, barrier layers, multiplication integration, and 2D and quasi-2D perovskites have all been conducted with reference to the stability issue. A significant body of research has recently been published on MA-free perovskite, which provides higher stability and efficiencies. PbI^+ unit vacancies within the perovskite lattice are present in d-HPs, or lead- and iodide – deficient HaPs, a recently discovered new family of perovskites that can be conceptualized as a bridge between 3D and 2D perovskites.

They are written as (A')3.48x(A)1–2.48x[$Pb_{1-x}I_{3-x}$], where A can be either methylammonium or formamidinium (FA^+). The following two large organic cations are reported as A': hydroxyethylammonium ($HO\text{-}(CH_2)_2\text{-}NH^{3+}$ or (HEA^+) and thioethylammonium ($HS\text{-}(CH_2)_2\text{-}NH^{3+}$ or (TEA^+), which do not follow the Goldschmidt tolerance factor. They show a 3D perovskite corner-shared $Pb_{1-x}I_{3-x}$ network that can be combined with a lead iodide deficient ($MAPbI_3$) or $FAPbI_3$ (FAPI) network. HEA^+ or TEA^+ can be inserted to produce d-MAPI-HEA and d-FAPI-TEA perovskites, respectively. The most important thing is that both systems' stability has increased, even though not much has been done to optimize them as thin films thus far. Similar structures have been reported based on the use of additional large cations, such as propylenediammonium, trimethylenediammonium, and ethylenediammonium. Hollow perovskites are the name given to this family of perovskites.

Current State of Efficiency in PSCs

PSCs have witnessed extraordinary advancements in efficiency, achieving conversion rates above 25% within just over a decade since their inception. Initially developed in 2009, these cells have rapidly progressed due to innovations in material synthesis and device architecture. The hybrid organic-inorganic perovskite structure, typically composed of $MAPbI_3$, has been pivotal in enhancing light absorption and charge carrier mobility. Recent studies have highlighted the advantages of

tandem configurations, where PSCs are paired with traditional silicon cells to create a dual-junction system that maximizes light utilization. This section will explore landmark achievements in efficiency and discuss the role of innovative fabrication techniques, such as solvent engineering and anti-solvent methods in improving the reproducibility and performance of PSCs. The growing interest in scaling up production methods without compromising efficiency is also a focal point, illustrating the potential of PSCs to compete with established photovoltaic technologies [7].

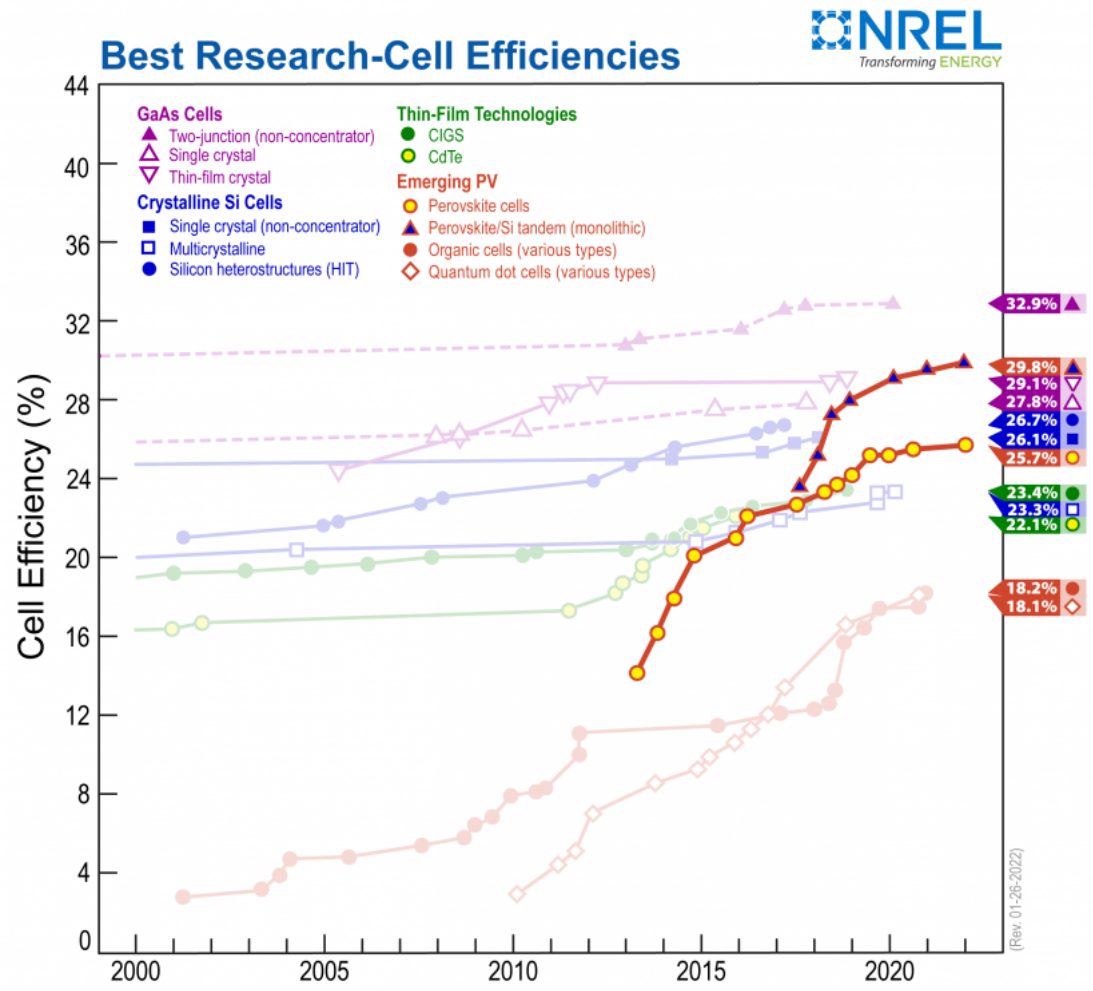

Figure 2. PCE at scale.

CHALLENGES IN STABILITY AND DURABILITY

The impressive efficiencies of PSCs come with a critical caveat: their stability and durability remain significant hurdles for commercial viability. Environmental factors, such as moisture, heat, and UV light have been shown to severely impact the operational lifespan of PSCs, leading to performance degradation. This section discusses the susceptibility of perovskite materials to humidity-induced degradation, Figure 2 where the absorption of water vapor can result in the formation of secondary phases that diminish electrical properties. Furthermore, thermal stability is a major concern, especially under prolonged exposure to high temperatures, which can induce phase transitions detrimental to performance. Emerging encapsulation strategies and protective coatings are being developed to shield PSCs from environmental stressors. Additionally, the importance of understanding the intrinsic instability of certain perovskite compositions will be highlighted, showcasing recent research aimed at identifying more robust material alternatives. Addressing these challenges is crucial for the long-term adoption of PSC technology in real-world applications.

COMPOSITIONAL ENGINEERING TECHNIQUES FOR EFFICIENCY IMPROVEMENT

Compositional engineering is a vital strategy for enhancing the efficiency of PSCs, allowing researchers to manipulate the material properties to achieve optimal performance. This section delves into the effects of varying the ratios of different cations, such as cesium, rubidium, and various lead substitutes, to optimize the photovoltaic properties of perovskites. By introducing mixed halide compositions, researchers have observed significant improvements in charge transport and light absorption. The role of additives, such as 2D perovskites and metal nanoparticles, in enhancing charge separation and reducing recombination losses will also be discussed. Innovations like the incorporation of 2D materials to stabilize the perovskite phase while enhancing performance have opened new avenues for research. Moreover, the application of machine learning and artificial intelligence to predict and optimize new material compositions will be explored, demonstrating its potential to accelerate the discovery of next-generation PSCs. This section will provide insights into how these compositional strategies are shaping the future of PSC technology [8].

IMPACT OF COMPOSITIONAL VARIATIONS ON STABILITY

Compositional variations in perovskite materials can significantly affect both their efficiency and stability, necessitating a comprehensive understanding of these relationships. This section focuses on how altering the composition of the perovskite layer influences its crystallographic structure and stability. For instance, changes in the halide ratio can dictate the thermal and moisture stability of PSCs, with certain combinations proving more resilient than others. Research has demonstrated that alloying strategies can mitigate common degradation pathways, enhancing the robustness of the perovskite layer under environmental stress. Furthermore, the role of ionic defects and their contribution to the degradation mechanisms will be examined, highlighting the importance of defect engineering in stabilizing perovskite structures. This section will also discuss the effects of varying the organic cation on phase stability and its correlation with long-term performance. By understanding the nuances of how compositional choices affect stability, researchers can design more durable PSCs capable of withstanding real-world conditions.

ENVIRONMENTAL IMPLICATIONS OF PEROVSKITE MATERIALS

The environmental impact of PSCs is an essential consideration as the technology progresses toward commercialization. This section evaluates the lifecycle of PSCs, including raw material extraction, manufacturing processes, and end-of-life management. While perovskites can offer substantial advantages in terms of energy conversion efficiency and lower production costs compared to traditional solar cells, concerns regarding the toxicity of certain elements, particularly lead, must be addressed. Recent advancements in the development of lead-free perovskite materials and their potential to minimize environmental risks will be examined. The section will also explore recycling strategies for perovskite materials, emphasizing the need for sustainable practices in the solar industry. By analyzing the overall ecological footprint of PSCs, this section aims to provide a balanced perspective on the sustainability of perovskite technology, advocating for responsible innovation in the renewable energy sector.

FUTURE DIRECTIONS IN PSC RESEARCH

The future of PSCs is filled with exciting possibilities, driven by ongoing research aimed at overcoming existing challenges and harnessing their full potential. This section outlines the key research avenues that are expected to shape the next generation of PSC technology. One promising direction is the development of tandem solar cells that combine perovskites with silicon or other emerging materials to achieve efficiencies beyond the limits of traditional technologies. Additionally, researchers are exploring advanced manufacturing techniques, such as large-scale printing and roll-to-roll processing, to facilitate cost-effective production. The integration of energy storage solutions with PSCs is another area of growing interest, enabling more efficient energy management in photovoltaic systems. The use of artificial intelligence and machine learning in material discovery and optimization is revolutionizing the design process, allowing for rapid advancements in perovskite technology. This

section will emphasize the importance of interdisciplinary collaboration and the need for strategic partnerships between academia, industry, and policymakers to propel PSCs into the mainstream market [10].

CONCLUSIONS

In conclusion, PSCs represent a transformative technology with the potential to reshape the future of renewable energy. This section summarizes the key findings from the manuscript, highlighting the impressive efficiency gains and the challenges related to stability and environmental sustainability. Recommendations for future research will include prioritizing the exploration of stable and non-toxic perovskite materials, enhancing encapsulation strategies to improve durability, and scaling up production methods. Collaborative efforts across disciplines will be essential to address the multifaceted challenges facing PSC technology. Furthermore, investment in public-private partnerships can facilitate the transition from laboratory-scale successes to commercial viability. By embracing a holistic approach that considers efficiency, stability, and environmental impact, the solar industry can unlock the full potential of PSCs, positioning them as a cornerstone of a sustainable energy future.

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