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Advancement Of Stable Carbon-Based Perovskite Solar Cellsusing Additive Engineering on Halide Perovskites

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ABSTRACT

Perovskite solar cells are an exciting new development in photovoltaic technology due to its low production costs and high efficiency in converting sunlight into power. However, they remain very unstable when subjected to environmental stresses such as moisture, heat, and ultraviolet light. Through the use of additive engineering to halide perovskite materials, this research aims to enhance the stability of carbon-based perovskite solar cells. As an affordable and environmentally friendly substitute for conventional metal electrodes, carbon-based electrodes provide superior chemical stability. In addition to reducing the cost of materials, they increase the lifespan of gadgets. The film's form, crystallinity, and defect passivation are improved in this work by adding several compounds to the halide perovskite structure. In order to stabilize the device, decrease ion mobility, and inhibit non-radiative recombination, these chemicals are crucial. Investigated here are the structural, optical, and electrical changes brought about by the incorporation of various elements into perovskite films, such as organic molecules, metal salts, and polymeric compounds. A more well-designed interface between the perovskite and carbon electrodes allows for more efficient charge transfer with reduced energy loss.Perovskite solar cells made of carbon are better suited for use in the long run since additive manufacturing considerably improves their performance and reliability. Perovskite solar systems that are steady, inexpensive, and environmentally beneficial might soon be available, as shown in this paper.

Keywords: ***Carbon-Based, Solar Cellsusing, Engineering, Perovskites***

INTRODUCTION

Due to the rapidly rising power consumption in everyday usage, there is a vital need for next generation sustainable, clean, and renewable energy sources. More efficient and strong energy sources are required to meet the increasing demand. The majority of the world's energy, over 80%, comes from non-renewable sources like coal, natural gas, fossil fuels, etc., which has devastating effects on the environment, including the release of greenhouse gases that cause climate change and a host of health problems. Energy is essential in the modern scientific and technological period, yet natural energy sources are finite and cannot be recycled. Every day, more and more people are calling for renewable energy sources that are more efficient and powerful. Solar, biomass, wind, and geothermal energy are some of the alternative energy sources that have recently attracted significant attention due to their efficiency, reliability, low cost, and renewable nature. One of the most effective renewable energy sources that may meet energy needs to a certain degree is the solar cell.

Perovskite Solar Cells: An Overview

Perovskite solar cells (PSCs) represent a significant improvement in photovoltaic technology during the last decade. These devices use a class of minerals known as perovskites, characterized by a common crystal structure similar to calcium titanium oxide ($CaTiO_3$). Perovskite materials in solar cells are predominantly organic–inorganic hybrid halides, defined by the chemical formula ABX_3, where ‘A’ indicates a monovalent cation (such as methylammonium, formamidinium, or cesium), ‘B’ denotes a divalent metal cation (usually lead or tin), and ‘X’ represents a halide anion (iodide, bromide, or chloride). This unique structure provides exceptional optoelectronic properties that make perovskites very suitable for solar energy conversion. A key advantage of perovskite materials is their remarkable light absorption capability. Slender layers of perovskite can efficiently absorb a wide range of sunlight, enabling the creation of lightweight and adaptable solar systems. Furthermore, perovskites have prolonged charge carrier diffusion lengths and low exciton binding energies, promoting the efficient separation and movement of electrons and holes inside the material. These properties improve power conversion efficiencies (PCEs), which have increased from around 3.8% in 2009 to over 25% in recent years, rivaling traditional silicon-based solar cells. The essential structure of a perovskite solar cell has many functional layers arranged in a specific order to enhance charge generation and extraction. The device typically consists of a transparent conductive oxide (TCO) layer, such as fluorine-doped tin oxide (FTO) or indium tin oxide (ITO), serving as the front electrode. The electron transport layer (ETL), often made of materials like titanium dioxide (TiO_2) or tin oxide (SnO_2), facilitates electron movement while preventing hole migration. The perovskite absorber layer is positioned above the electron transport layer and is essential for capturing sunlight and generating electron-hole pairs. The hole transport layer (HTL), positioned above the perovskite layer, often comprises organic materials such as Spiro-OMeTAD or inorganic options such nickel oxide (NiO). Ultimately, a back electrode, usually made of metals like gold or silver, completes the setup. Perovskite solar cells may be classified into many architectures based on their structural configuration, including mesoporous, planar, and inverted (p-i-n) structures. In mesoporous structures, a porous scaffold, often TiO_2, underpins the perovskite layer, hence enhancing charge separation and transport. Planar designs eliminate the mesoporous layer, optimizing production and enhancing compatibility with flexible substrates. The inverted design modifies the arrangement of electron and hole transport layers, often improving device stability and reducing hysteresis effects. Each architectural design has unique advantages and challenges, with ongoing research aimed at optimizing these structures for improved efficiency and resilience.

\Despite their remarkable efficacy, PSCs have several challenges that hinder their broad commercialization. A major worry is their instability in response to environmental factors such as moisture, oxygen, heat, and ultraviolet (UV) light. The organic components of hybrid perovskites demonstrate increased vulnerability to degradation, leading to rapid decline in device performance over time. The presence of lead in several high-performing perovskite compounds poses concerns about environmental safety and toxicity. Researchers are rigorously exploring lead-free alternatives, such as tin-based perovskites, despite their current lower efficiency and stability. Another issue associated with perovskite solar cells is the presence of current-voltage hysteresis, which undermines the accuracy of efficiency evaluations and indicates intrinsic challenges in charge transport and ion migration. This phenomenon is often attributed to defects in the perovskite layer, interface inconsistencies, and ionic migration in the presence of an electric field. Addressing these difficulties requires precise material engineering, interface optimization, and advanced manufacturing techniques. In recent years, significant progress has been made to overcome these limitations using several approaches, including compositional engineering, interface modification, and additive engineering. Additives, such as small molecules, polymers, or inorganic salts, are included into the perovskite precursor solution to enhance film morphology, improve crystallinity, and reduce defect density. These modifications provide superior charge transfer, less recombination losses, and enhanced stability. Moreover, the use of carbon-based electrodes instead of expensive noble metals has attracted attention as a cost-effective and resilient alternative, particularly for large-scale and printable solar cell technologies.

Perovskite solar cells additionally provide advantages concerning manufacturing methodologies. Unlike traditional silicon solar cells that need high-temperature and energy-intensive processes, perovskite solar cells (PSCs) may be fabricated using low-temperature, solution-based technologies such as spin coating, doctor blading, and inkjet printing. These methods enable the production of large-area devices at lower prices, making perovskite solar cells especially attractive for commercial use. Furthermore, their compatibility with flexible substrates presents prospects for innovative applications, including as wearable electronics, building-integrated photovoltaics (BIPV), and portable power sources. A significant benefit of perovskite solar cells is its compatibility with tandem solar cell applications. Combining perovskites with other photovoltaic technologies, such as silicon or CIGS (copper indium gallium selenide), might surpass the efficiency limits of single-junction solar cells. Perovskites may be engineered with tunable bandgaps, allowing them to absorb different portions of the solar spectrum when configured in tandem. This approach has shown above 30% efficiency in laboratory settings, highlighting the transformative potential of PSCs in renewable energy. Perovskite solar cells represent an emerging and very promising photovoltaic technology capable of revolutionizing the solar energy industry. Their exceptional optoelectronic properties, high efficiency, low production costs, and versatility make them strong contenders for next-generation solar technologies. However, challenges related to stability, toxicity, and scalability must be addressed before achieving widespread commercialization. Ongoing research efforts focused on material innovation, device engineering, and sustainable design are expected to enhance the performance and dependability of PSCs, hence enabling their integration into future energy systems.

First Generation of Solar Cells

The First Generation of solar cells has a single P-N junction of crystalline silicon. The power conversion efficiency of this kind of solar cell is 27% at the laboratory size and 24% at the commercial scale. The theoretical efficiency limit for the same solar cell, as determined by Shockley and Queisser, is 31%. Currently, about 85% of photovoltaic technology relies on this form of solar cell. Furthermore, although first-generation solar cells exhibit excellent efficiency and longevity, they are costly owing to their intricate manufacturing process and installation requirements.

Figure 1 Generation of Photovoltaic solar cells with various materials blend and technology

Second Generation of Solar Cells

The Second Generation of solar cells include amorphous silicon (a-Si), microcrystalline silicon, polycrystalline silicon, cadmium telluride (CdTe), copper indium gallium selenide (CIGS), and gallium arsenide (GaAs), among others. The majority of second-generation solar cells use thin film technology, with thicknesses ranging from a few nanometers to micrometers. Table (1) delineates the efficiency of several types of second-generation solar cells.

Efficiency and market share of various solar devices

Table 1. Efficiency And Market Of Some Photovoltaic Devices

Based Device	Efficiency	Share PV market in 2015
GaAs	28%	-
CIGS	21.5%	37%
CdTe	21.7%	36%
a-Si	13.4%	27%

All these solar cell types exhibit more flexibility than first-generation solar cells; nevertheless, the intricate manufacturing process of CIGS and the elevated cost of GaAs restrict the commercialization of these high-efficiency solar cells. These solar cells exhibit reduced durability compared to first-generation solar cells and also raise environmental concerns.

Third Generation of Solar Cells

This kind of solar cells is designed as thin film deposits on a supporting substrate or as quantum dots. Organic solar cells, polymer solar cells, dye-sensitized solar cells (DSS), and multi-junction solar cells exemplify the third generation of solar technology. The National Renewable Energy Laboratory (NREL) confirmed that organic, dye-sensitized solar (DSS), and quantum dot solar cells had power conversion efficiencies (PCEs) of 11.1%, 13.4%, and 9.9%, respectively. These solar cells may be produced rapidly within a few hours, making them more economical than the previous two generations of solar cells.

Fourth Generation of Solar Cells

Fourth Generation solar cells consist of a mix of organic and inorganic materials, therefore referred to as hybrid solar cells. The solar cells primarily use perovskite materials and represent the latest advancement in fourth-generation photovoltaic technology. In only six years, its power conversion efficiencies (PCEs) rose from 3.18% to 23%, indicating its significance and quick advancement with organic-inorganic perovskite materials. However, because to the presence of lead components and insufficient stability, it has yet to be marketed.

Carbon-Based Perovskite Solar Cells (C-PSCs)

To replace the costly noble metals used as back electrodes in traditional perovskite solar cells, carbon-based perovskite solar cells (C-PSCs) have recently gained popularity. The carbon materials used as the counter electrode in C-PSCs include graphene, carbon nanotubes (CNTs), graphite, and carbon black. These materials are ideal for improving the longevity and economic feasibility of perovskite solar cells because of their cheap cost, strong electrical conductivity, chemical stability, and hydrophobicity, among other benefits. Fixing the problem of stability over time is a major driving force behind using carbon electrodes instead of metal ones. Device deterioration may occur when conventional metal electrodes diffuse into the perovskite layer due to thermal or operational stress. Carbon, on the other hand, is chemically inert and hence improves the device's stability since it reacts less readily with perovskite components. Another important aspect in reducing environmental deterioration is the improved resistance to moisture intrusion that carbon electrodes provide owing to their hydrophobic characteristics. A hole transport material (HTM)-free design is often used to construct C-PSCs, which further simplifies device production and saves cost. Here, the carbon electrode serves as a collector of holes by coming into direct touch with the perovskite layer. Organic hole transport materials such as Spiro-OMeTAD are no longer necessary; these materials are unstable, costly, and vulnerable to moisture and dopant degradation, all of which may reduce their long-term effectiveness. Consequently, C-PSCs are sometimes called "fully printable" or "low-cost" solar cells since they can be made utilizing scalable processes like screen printing and doctor blading.

RESEARCH METHODOLOGY

The photovoltaic industry has recently embraced organic-inorganic halide perovskite solar cells (PSCs) as a leading candidate for enhanced efficiency (Min et al., 2021). Halide perovskites are often represented by the generic formula ABX3, with A being a monovalent cation such as methylammonium iodide (CH3NH3I), Formamidinium iodide (CH(NH2)2I), or cesium (Cs+) situated at each of the eight corners of the unit cell. At its core, B is a divalent metal cation from the carbon family (Pb2+, Sn2+, and Ge2+), whereas in its six-face center, X is a monovalent halogen anion, for example X= Cl-, Br-, or I-. Perovskite materials are very attractive for PSC research because to their strong light absorption over a broad range of infrared-visible spectra (Saparov & Mitzi 2016; Xiao et al. 2014), rapid carrier mobility (Guse et al. 2016), and low exciton recombination rate (Miyata et al. 2015). Electron transport layer (TiO2), perovskite layer (PLV), hole transport layer (HTL), and metal contact make up a typical PSC. One drawback of this approach is the high cost and fragility of organic HTM, such as Spiro-OMeTAD. Recent efforts, however, have focused on finding alternatives to the expensive Spiro-OMeTAD HTM for PSCs (Pham et al. 2018a; Pham et al. 2018b). On top of that, PSCs may not work as well with metal electrodes like Au/Ag. Excessive vacuum is required for the processing of these precious metals, which adds to their high price tag. Their gradual corrosion in reaction with halogen ions shortens the PSCs' storage life (Zhang et al. 2015). This suggests that PSC commercialization is going to be challenging down the road. The good news is that it is not necessary to consume HTM for the HTM free carbon-based PSC to function effectively. In an oxygen-rich atmosphere, CH3NH3PbI3 degrades quickly. Perovskite solution is dropped onto surfaces that include m-TiO2/m-ZrO2/Carbon Counter Electrode (CE), as shown in Figure 2 (a). In carbon-based perovskite, Figure 2 (b & c) shows a schematic of CPSCs, energy levels, and hydrogen bond interactions with 5-AVAI. The 5-AVAI molecule forms hydrogen bonds with perovskite halides (CH3NH3PbI3) via the carboxylate (-COO-) and amino (-NH3+) functional groups [(O-H----I) and (N-H I)]. According to Li et al. (2015b), perovskite materials have a longer shelf life because of this interaction involving hydrogen bonds

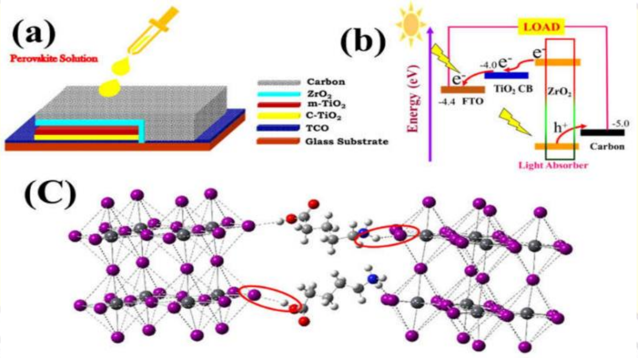

Figure 2 Schematic presentation of (a) CPSC, (b) energy level and(c) hydrogen bond interaction between CH3NH3PbI3 and 5-AVAI

We used a perovskite solution containing a 5-AVAI cation in a triple mesoscopic PSC structure for our investigation. In comparison to the pure perovskite film, the additive-based one exhibits less PbI2 phase development. To study the noticeable variation in the perovskite with 5-AVAI cation addition, we used X-ray diffraction (XRD), ultraviolet-visible (UV-Vis), photoluminescence (PL), and Fourier transform infrared (FTIR) spectroscopy. The additive and perovskite establish a hydrogen bond, which improves the device's performance by passingivating surface imperfections. A maximum efficiency of 6.6% in power conversion is shown by the CPSC device. After testing the gadget at room temperature and humidity, researchers found that it had an exceptional shelf life of 75 days. Perovskite solar cells that are stable are made possible by adding 5-AVAI cation. According to Li et al. (2015b), perovskite materials have a longer shelf life because of this interaction involving hydrogen bonds

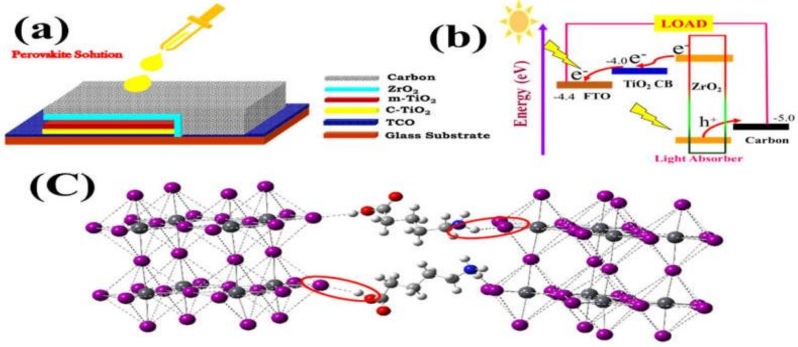

Figure 3 Schematic presentation of (a) CPSC, (b) energy level and(c) hydrogen bond interaction between CH3NH3PbI3 and 5-AVAI

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RESULTS AND DISCUSSION

Optical Microscope Analysis

Within this research, we examined perovskite films under ambient conditions and examined a 5-ammonium valeric acid iodide addition to the perovskite precursor. Under the metallurgical microscope, the perovskite layers' morphology was examined. Figure 4 (a) and (b) show the layers of CH3NH3PbI3 before preparation and three hours after preparation, respectively. Pinholes and other forms of poor film formation are seen in the as-prepared perovskite layer that did not include any addition. The perovskite coating showed signs of degradation after three hours under ambient conditions, with the production of a needle-like structure. This structure suggests that PbI2 was formed from CH3NH3PbI3. The perovskite layer with 5-AVAI additions exhibits big grains, uniformity, and the absence of pinholes in its as-prepared state. Figure 5 (a & b) shows that the perovskite layers with 5-AVAI added have a longer shelf life after three hours at room temperature, as no needle-like structure is visible. The presence of 5-AVAI cation in the aged perovskite film with an expanded grain boundary indicates that the cation has a substantial impact on the crystallization process and the morphology of the perovskite film creation.

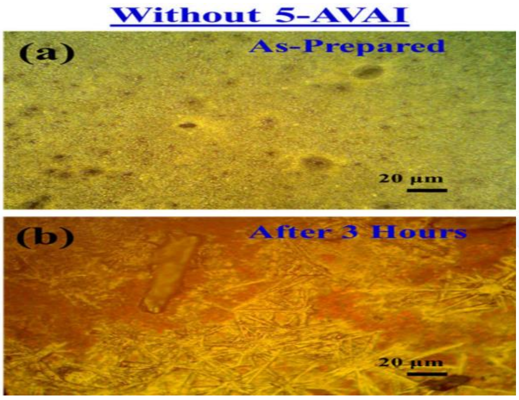

Figure 4 Optical microscope image of (a) As-prepared and (b) after 3 hours pristine CH3NH3PbI3 layer

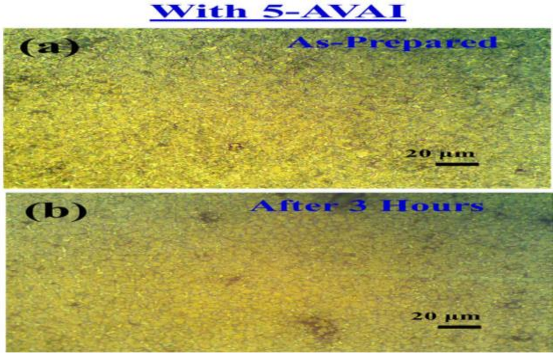

Figure 5 Optical microscope image of (a) As-prepared and (b) after 3 hours of with 5-AVAI additive

Powder X-ray Diffraction (PXRD) Analysis

Figure 6 displays the X-ray diffraction pattern that explained the structural characteristics of the perovskite films in their as-prepared state. In the tetragonal perovskite crystal structure, the (110), (112), (211), (202), (220), (310), (312), (234) and (314) planes are equivalent to the diffraction peaks at 2θ values of 14.1°, 20.07°, 23.5°, 24.53°, 28.47°, 31.88°, 35°, 40.76°, and 43.2°. The 5-AVAI addition improves the perovskite film's quality, which in turn raises the crystallinity of the film (14.1°). A drop from 0.1791° to 0.0768° in the Full Width at Half-Maximum (FWHM) of the (110) diffraction peaks suggests that the 5-AVAI additive may chemically bridge the perovskite structure, enhancing the crystallization of perovskite films with larger grain boundaries and inducing crystal growth orientation relative to pure perovskite film. The perovskite film's 5-AVAI additive reduces the prominence of the PbI2 (12.64°) peak. Because of this change, the device's stability and photovoltaic performance are both enhanced.

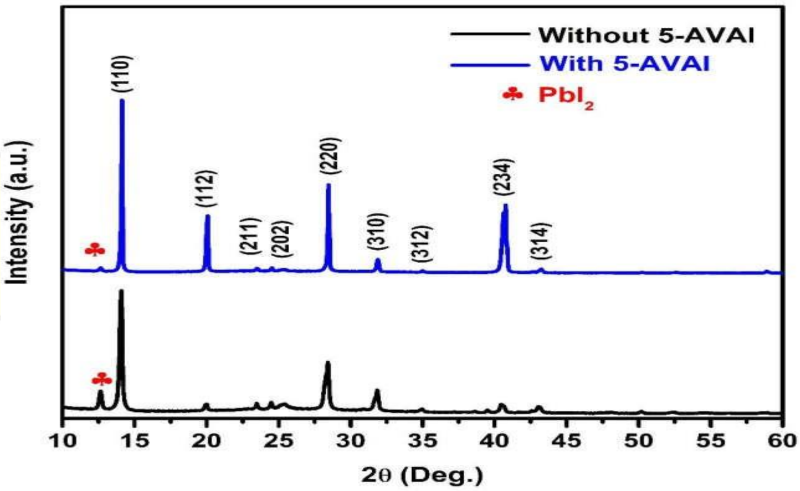

Figure 6 X-ray diffraction pattern of perovskite film with and without 5-AVAI additive

Fourier Transform Infrared Spectra (FTIR) Analysis

The interaction between 5-AVAI and MAPbI3 was further investigated by comparing the Fourier Transform Infrared Spectra (FTIR) of perovskite films with and without 5-AVAI films. The results are shown in Figure 7 (a & b). For 5-AVAI, MAPbI3, and MAPbI3-5AVAI, the N-H stretching frequencies are 3174 cm-1, 3056 cm-1, 3192 cm-1, 3135 cm-1, 3152 cm-1, and 2960 cm-1, correspondingly. As a result of the interaction between I- and -COOH, the C=O stretching frequency of 5-AVAI and MAPbI3-5AVAI is changed from 1704 cm-1 to 1734 cm-1 when 5-AVAI is added. Additionally, the perovskite coatings may be securing themselves against moisture by this effect. The results show that the N-H and C=O stretching frequencies, caused by 5-AVAI's amine and acid functional groups, affect the interaction between MAPbI3 and 5-AVAI in the perovskite film.

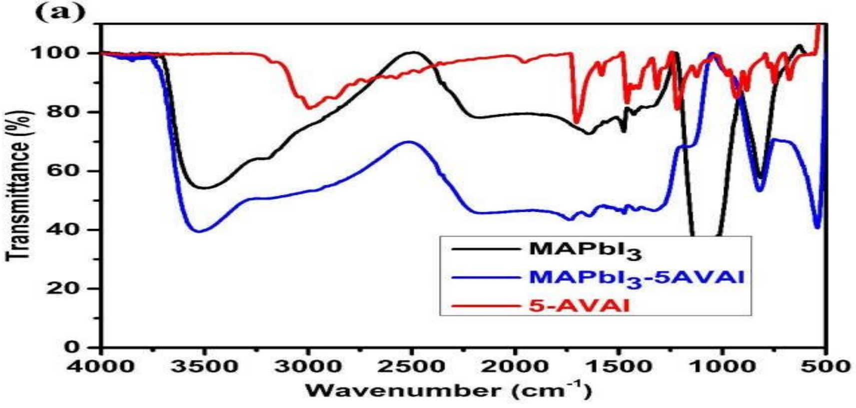

Figure 6 (Continued)

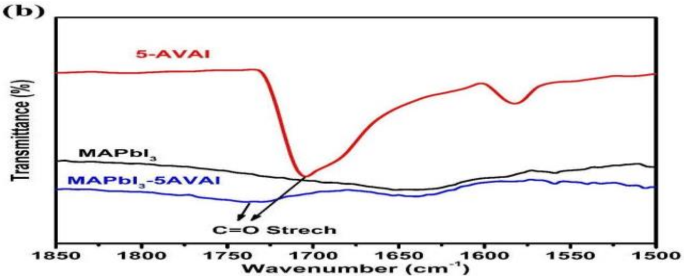

Figure 7 (a) FTIR spectra of 5-AVAI, MAPbI3 and MAPbI3-5AVAI(b) Enlarged FTIR spectra of 5-AVAI, MAPbI3 and MAPbI3-5AVAI

CONCLUSION

The reliability and efficiency of the CPSC device and perovskite layer are the primary foci of this thesis. Halide perovskites were enhanced in performance and stability by adding additives. Crystallinity, crystal size, defect site minimization, and growth along the chosen orientation are all enhanced in the additively formed perovskite layer. A hydrogen link between the additives and the MA cation in the perovskite structure further stabilized the perovskite layer. The device's photovoltaic performance is enhanced because this weak contact slows down crystallization and grows with fewer crystal grains. This section discusses an intriguing property of the additive-added perovskite absorber based CPSC device Solar energy, renewable energy sources, energy demand, and related topics including the photovoltaic effect and new generations of solar cells have all been covered. A quick overview of the PSC technology's working principle, several kinds of designs and their components, and the necessary steps to be ready is provided. Everyone is familiar with the basics of perovskite structure, how to prepare them, and how to fabricate devices using them. In the first chapter, PSC technology is covered extensively, covering the perovskite layer's defining characteristics, device designs, and potential future applications. Chapter states that the CPSC device maintains a shelf-life efficiency of more than 90% under ambient air conditions for 75 days. Crystallization is superior in the perovskite layer that contains 5-AVAI additions compared to the pure perovskite layer.

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