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CsPbX3 PEROVSKITES, A TWO-TIER MATERIAL FOR HIGH-PERFORMANCE, STABLE PHOTOVOLTAICS

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Abstract

The inorganic CsPbX3 perovskite has received a lot of attention due to its high carrier transport efficiency and high thermal stability. However, solution-processed CsPbX3 perovskite solar cells' PCE is still significantly lower than that of their hybrid counterparts. Their devices' functionality is hampered by two main factors: insufficient film thickness and unwanted phase transition. Here, we demonstrate that the well-known solubility limitation for Cs precursors may be circumvented for the production of high-quality CsPbX3 perovskite films of considerable film thickness by using a novel precursor pair consisting of cesium acetate (CsAc) and hydrogen lead trihalide (HPbX3) (500 nm). To further encourage reduced-dimensional perovskite production, we added a small quantity of phenylethylammonium iodide (PEAI) to the solution. The resulting quasi-2D perovskites greatly lowered the trap density in the film by inhibiting unwanted phase transition. Using this method, we reported a 12.4 percent PCE for reduced-dimensional a-CsPbI3 perovskite photovoltaics, which is the best to date and has significantly longer performance lifetime than previous methods.

Introduction

Because of their excellent photophysical properties, organic-inorganic hybrid perovskites (CH3NH3PbX3) have recently emerged as the most promising new generation photovoltaic material [1-3]. However, their organic components are highly volatile, making them thermally unstable at high temperatures. Inorganic cesium lead halide perovskites (CsPbX3) have attracted a lot of interest as a potential solution to this issue because of their high thermal stability and excellent carrier transport features. Still, the performance of photovoltaic devices lags significantly behind that of their hybrid analogue, CH3NH3PbX3. High-quality CsPbX3 perovskite films with significant film thicknesses (>400 nm) have yet to be fabricated using the solution processing approach [4-7].

CsPb(I1-xBrx)3 (x 0.5) perovskites are thermodynamically unstable in their black cube phase at ambient temperature because of their high iodide content. In order to increase PCE, narrower band gap iodide-rich CsPb(I1-xBrx)3 perovskites must be used as absorbers. However, under normal conditions, the black cube phase (a-CsPbX3) of iodide-rich perovskites spontaneously transforms into the yellow orthorhombic phase (d-CsPbX3) of a non-perovskite. Stabilizing a-CsPbI3 perovskite at ambient temperature via nanocrystal surface engineering and bication two-dimensional (2D) ethylenediamine perovskite components yields a record PCE of 11.8% for all-inorganic perovskite solar panels. High-efficiency a-CsPbX3 perovskite solar cells were fabricated using a face single-step deposition approach using the highly soluble precursors cesium acetate (CsAc) and hydrogen lead trihalide (HPbX3) [8-16].

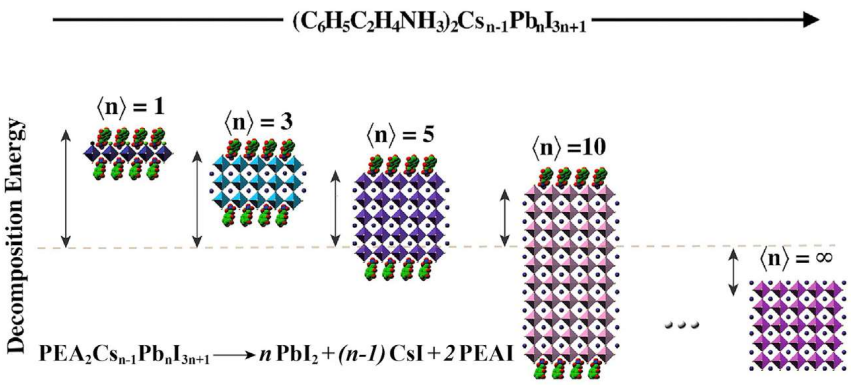

Figure 1. Crystal configuration of CsPbX3 Perovskites.

Experimental Method

This experiment utilized chemicals from Sigma-warehouses and Aldrich's without further purification. HPbI3 crystals were grown using anti-solvent vapor-assisted crystallization, and precursor solutions were generated by dissolving HPbI3 and hydrogen lead trihalide crystals in anhydrous DMSO solvent. The resulting solution was heated at 80°C in a toluene vapor atmosphere overnight. The HPbI3 powder was dried under vacuum at 80°C for 10 hours [19]. PEA2Csn-1PbnX3n+1 solutions were created by dissolved HPbX3, CsAc, and PEAX in DMSO and filtered. The films were annealed at 100°C for 30 minutes for improved crystallization. Pre-patterned ITO glass substrates were cleaned and subjected to a 10-minute UV zone treatment. Coating an ITO substrate with an 80-nanometer thick SnO2 electron transport layer required spinning a colloidal SnO2 nanocrystal solution and annealing it at 200°C for 30 minutes at room temperature. The perovskite absorber was placed onto the SnO2 substrate [20].

The steady-state open-circuit voltage (Voc) and steady-state short-circuit current (Jsc) were determined using a Keithley 2400 instrument. The photovoltaic EQE spectra were acquired using a method documented in the literature. Stability tests were conducted in a controlled laboratory setting at room temperature and relative humidity of 20% to 5% [21].

Characterization

The PL spectra were captured using a fluorometer made by Fluorolog-Horiba. Exciting the equivalent perovskite samples at 300 nm allowed for time-resolved PL measurements to be conducted. Using a Lambda 950 UV-visible spectrophotometer, we measured the absorption spectra of CsPb(I1-xBrx)3 perovskite and quasi-2D perovskite films. Field-emission SEM (JEOL, JSM-7500F) at an acceleration voltage of 1 kV was used to evaluate the surface morphology of perovskite films. The FEI Nova dual beam, focused ion beam system, combined SEM and gallium ion beam apparatus was utilized to create the cross-section SEM pictures. Using Cu Ka radiation (l = 1.5406 Å) and an XRD (Bruker AXS GmbH, BrukerD8 FOCUS), we were able to get crystallographic data [22].

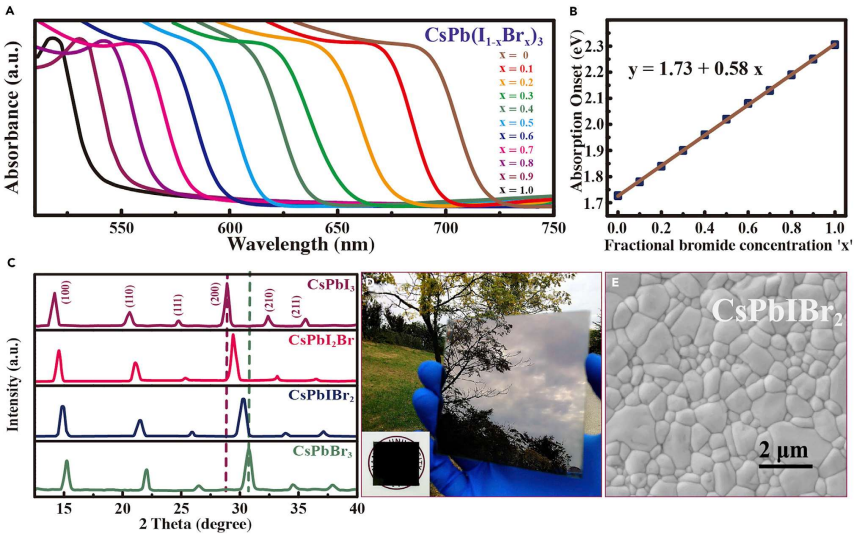

Figure 2. CsPbX3 is an inorganic perovskite film with different nanocomposites, characterized by absorbance spectra, optical band gap plots, X-ray diffraction patterns, and a mirror-like perovskite film coated on FTO glass. Its morphology is similar to other CsPbX3 films.

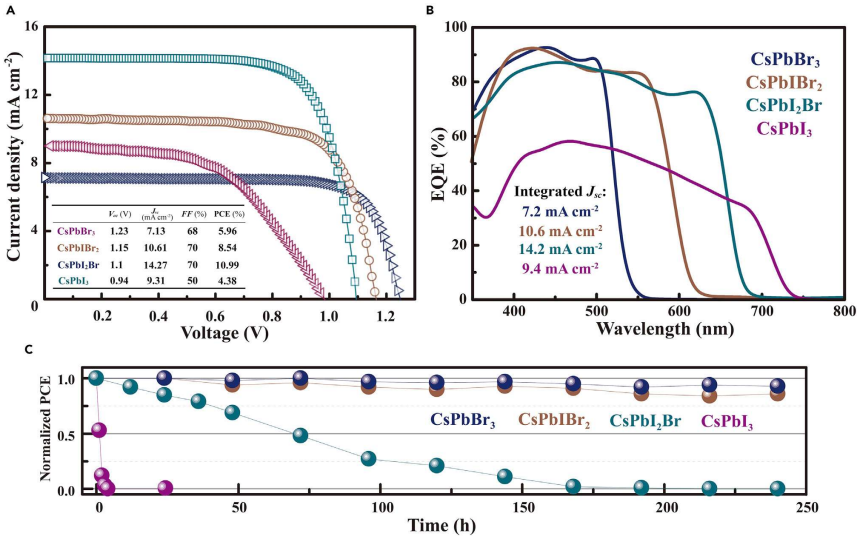

Figure 3. CsPbX3-based solar cells exhibit high performance, with J-V characteristics, EQE spectra, and performance evolution under ambient atmosphere.

Results & Discussion

Research has shown that lead acetate (PbAc2) is a suitable precursor for producing high-quality CH3NH3PbI3 films. A new precursor pair, HPbX3, was used to produce homogeneous and ultra-smooth films. The mirror-like coating is made of inorganic CsPbX3 cubic phase perovskite with a deep black hue [1-10]. The band-gap tuning of inorganic perovskites, CsPb(I1xBrx)3, was achieved by varying the molar ratio of HPbBr3 to HPbI3. The resulting films' detailed crystalline structures were studied using XRD, and the film morphology was investigated using scanning electron microscopy (SEM).

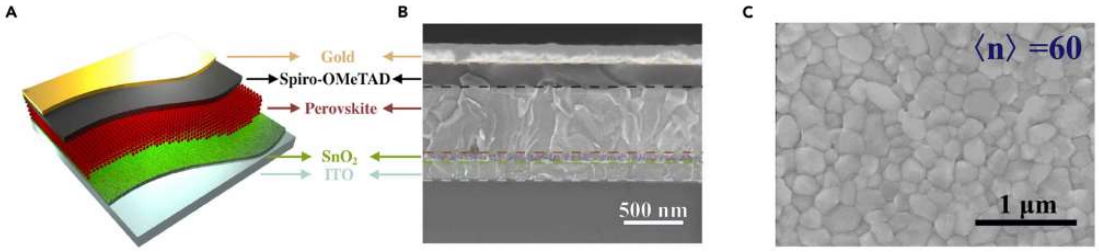

Figure 4. Quasi-2D perovskite-based devices exhibit photovoltaic performance, using PEA2Csn-1PbnX3n+1 absorbers and SEM images.

The optimized device performance for CsPbBr3, CsPbIBr2, CsPbI2Br, and CsPbI3 perovskites was optimized. The best PCE based on CsPbI2Br perovskite achieved 10.99% efficiency, outperforming the best vacuum deposited CsPbI2Br solar cells. The black cubic phase of narrower-band-gap iodide-rich CsPb(I1-xBrx)3 (x 0.5) perovskites must be stabilized to develop more efficient inorganic perovskite solar cells. The quasi-2D technique is a flexible way to improve CsPbX3 perovskite device stability and performance [11-20].

Conclusion

A simple single-step deposition approach synthesizes resilient ligand-stabilized a-CsPbX3 perovskites for high efficiency inorganic perovskite solar cells. The method overcomes solubility limitations and increases performance stability by inhibiting undesired phase transitions. This breakthrough enables commercial scale, low-temperature roll-to-roll production of flexible inorganic perovskite solar cells.

Conflicts of Interest: There are no potential conflicts of interest with the writers. The process of gathering information, analysing it, writing it up, and deciding if the findings should be made public.

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