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Advancements in Solution-Processed Perovskite Solar Cell Surface States and Interface Optimization

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KEYWORDS

Perovskite solar cells (PSCs), Photovoltaic applications, Solution procedures, Surface and interface properties, Fabrication methods.

Abstract

Perovskite solar cells (PSCs) have shown significant growth in power conversion efficiency, increasing from 3.8% to over 20%. PSCs are chemically similar to dye-sensitized solar cells, using a medium containing hole transporting materials (HTMs) and light-absorbing components to sensitize mesoporous TiO2. However, PSCs are particularly beneficial for photovoltaic applications due to their long photocarrier diffusion lengths and surface states that can serve as recombination sites. Affordable production of PSCs is crucial, and the availability of solution procedures is a critical factor. High PbI2 concentration is essential for better performance, and the high efficiency of PSCs is heavily dependent on surface and interface properties. First-principles computations show that all four surface aspects of tetragonal MAPbI3 have two major phases, with the former being more stable under thermodynamically equilibrium conditions and the latter being vacant- or flat-type terminations. Flat terminations are advantageous for PSC performance in a PbI2-rich environment, as they can amplify the extended carrier lifetime and facilitate hole transport to HTMs.

Introduction

Converting sunlight into electricity is crucial for sustainable economic growth through renewable energy without harming the environment [1]. Organometal halide perovskite solar cells have been extensively studied due to their rapid increase in power conversion efficiency. In 2009, Miyasaka et al. initially used CH3NH3PbX3 (MAPbX3, X = Br, I) as a light absorber in liquid-based dye-sensitized solar cells (DSSCs) [2-5]. The stability of implanted MAPbI3 in liquid electrolyte was enhanced by using robust hole transporting materials (HTMs). Moreover, perovskite solar cells (PSCs) that demonstrated long-term stability had an enhanced efficiency of 9.7%.3 Within 5-6 years, the power conversion efficiencies of perovskite solar cells have risen from 3.8% to over 20% [6].

The quick growth can be seen as unique characteristics of organo-lead halide perovskites for solar purposes when compared to traditional DSSCs. One main benefit is their high light absorption capacity across a wide spectrum, allowing for a thinner sensitive layer [7]. The optical absorption coefficient of MAPbI3 exceeds 105 cm-1 in the short wavelength range [8]. The organolead halide perovskites have lengthy diffusion lengths of 1 μm or more for both charge carriers, which is quite intriguing [9]. The exceptional intrinsic characteristics of organolead halide perovskites are facilitated by their high mobility and slow recombination rate of holes and electrons [10]. Photoexcited electron-hole pairs behave as free carriers rather than following the commonly recognized exciton model [11]. The primary relaxation process observed in femtosecond transient absorption spectroscopy is the recombination of free electrons and holes [12]. The exceptional optoelectronic properties are explained by their electronic structures, which consist of a proper band gap, significant transition dipole moment, low carrier effective masses, and shallow defect levels present even at surfaces or grain boundaries. The lack of extra midgap states reduces carrier traps and nonradiative recombination centers, allowing for prolonged carrier delocalization and resulting in an extended diffusion length. Surface state energy levels are crucial and the primary focus of this Account [13].

Solution techniques are extremely popular due to their cost-effective manufacturing. PSCs share parallels in device compositions with DSSCs, as both contain light-absorption components positioned between carrier-transfer mediums such mesoporous-TiO2 (mpTiO2). An initial one-step approach, such as spin coating, was used to deposit perovskite components onto a carrier-transfer layer [14]. A two-step process is used to efficiently produce high-performance cells. First, PbI2 is deposited

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from a solution onto a mesoporous TiO2 film. Then, it is converted into MAPbI3. We assume that a high concentration of PbI2, known as the PbI2-rich growth condition, benefits the surfaces of MAPbI3, TiO2/MAPbI3, and HTM/MAPbI3 interfaces, enhancing the transit of photoexcited carriers [15].

This Account examines the electrical properties, specifically surface states, of several terminations of tetragonal MAPbI3 surfaces under varying growth conditions, which correspond to diverse chemical potentials, by first-principles calculations. Most of the results have been documented in our previous article [16]. The surfaces given are suitable interface models of MAPbI3/HTMs, with spiro-OMeTAD (2,2′,7,7′-tetrakis(N,N-di-p-methoxyphenylamine)-9,9′-bifluorene) representing them due to their weak interactions. Recommended characteristics for optimal PSC performance will be proposed, leading to stable terminations and surface electronic states [17]. Future potential for theoretical surface and interface investigations are discussed based on the experimental findings [18].

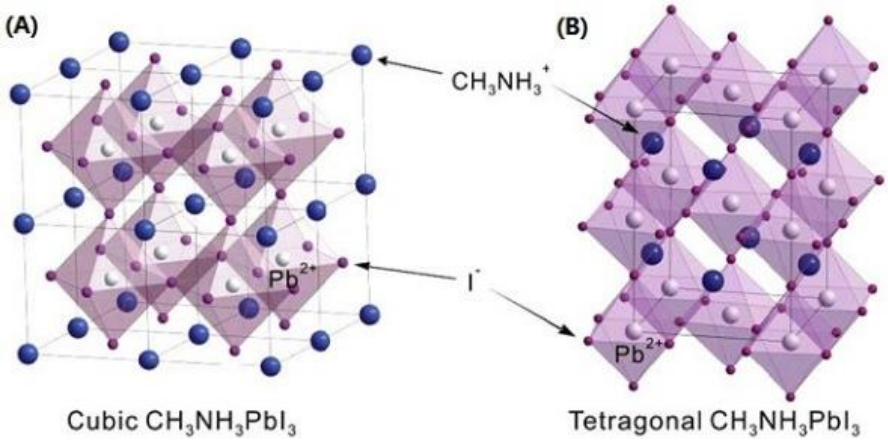

Figure 1. MAPbI3 with (A) cubic phase and (B) tetragonal phase.

Materials and Method

The ITO/glass substrates were treated with UV-O3 for 20 minutes before spin coating PEDOT:PSS at 5000 rpm for 40 seconds [19]. The substrates were then annealed at 150 °C for 10 minutes in air to manufacture the device. The MAPbI3 film, used as a light harvester, was applied using four distinct processes. The precursor solutions were agitated at a temperature of 60 °C for almost 2 hours. 70 units of N-cyclohexyl-2-pyrrolidone (CHP) were combined with 0.93 ml of a solution containing 35% by weight of MAPbI3 in dimethylformide (DMF), along with CH3NH3I and PbI2 in equal molar amounts. This mixture was then spin-coated onto PEDOT:PSS at 5000 rpm for 50 seconds and annealed at 100 °C for 10 minutes in a glove box filled with nitrogen. The solution containing MAPbI3–DMF precursor (30, 35 wt%) was applied onto PEDOT:PSS using spin coating at 4000 rpm for 30 seconds. Subsequently, 0.3 ml of chlorobenzene (CB) was rapidly added to the spinning wet MAPbI3 films after 6 seconds of the spin coating process. The films were then annealed at 100 °C for 10 minutes in a N2-filled glove box [20]. The PbI2-DMF precursor solution was spin-coated onto PEDOT:PSS at 2000 rpm for 20 seconds at 70 °C. Subsequently, a 20 mg/ml MAI-2-propanol precursor solution was spread over the PbI2 film when it turned cloudy [21]. The MAI solution was allowed to wet the PbI2 film for 20 seconds, followed by annealing at 70 °C for 10 minutes and then at 100 °C for 90 minutes in a N2-filled glove box. The deposition process for the PbI2 film is identical to the IFF approach. The PbI2 film was submerged in a 10 mg/ml MAI-2-propanol precursor solution for 60 seconds in the air [22]. The damp MAPbI3 film was washed with 2-propanol and the remaining solvent was rapidly eliminated using a N2 blow gun. The MAPbI3 film was quickly cooled to room temperature after deposition [23]. PC61BM, a solution containing 20 mg/ml in CB, was spin-coated onto MAPbI3 at 700 rpm for 60 seconds in a glove box sealed with nitrogen. Bathocuproine (BCP, Alfa) and silver (Ag) were placed onto the PC61BM layer using thermal evaporation in a vacuum of 10-6 Torr. The planar hybrid perovskite solar cells feature a structure consisting of ITO/PEDOT:PSS (30 nm)/MAPbI3 film [24].

Characterization

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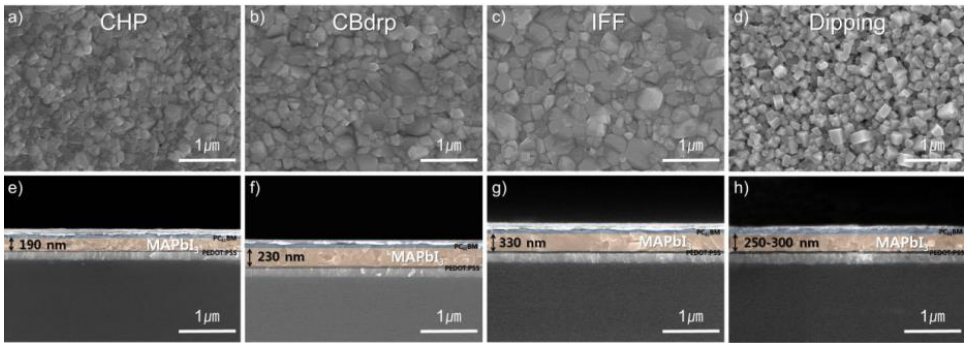

Figure 2. SEM images of deposited MAPbI3 films on PEDOT:PSS/ITO substrate.

The study used a SEM-3000 COXEM India microscope to capture SEM images of MAPbI3 films on a PEDOT:PSS/ITO substrate [25]. X-ray diffraction patterns were analyzed using Model 3010 ANALYTICAL TECHNOLOGIES India instrument [26].

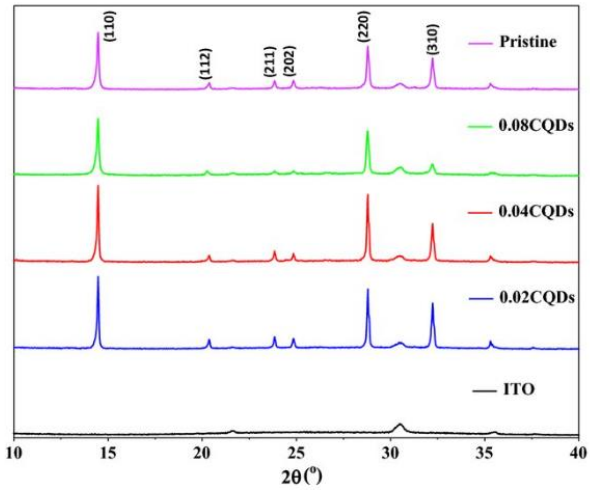

Figure 3. XRD- pattern of MAPbI3 films on PEDOT:PSS/ITO substrate.

UPS data was collected using an AXIS ULTRA DLD instrument. Fourier-transform infrared spectroscopy was conducted using a LABTRONICS India LT-4101 analyzer. The devices J-V characteristics were measured using a Keithley 4200 instrument under 100 mA/cm^2 illumination [27]. Consonant-vowel analysis was performed using an Agilent 4284A accuracy LCR meter. Time-resolved photoluminescence (TRPL) measurements were conducted using a mode-locked Ti:Sapphire laser. The PL lifespan was observed using a picosecond streak camera [28].

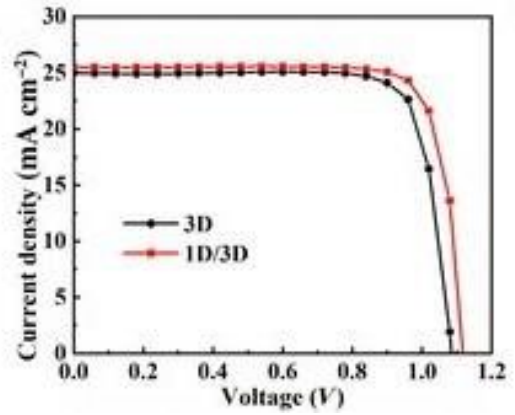

Figure 4. J-V characteristics of MAPBI3 films on PEDOT:PSS.

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Result and Discussion

The study investigates the morphology of various films and varies depending on the annealing duration. The crystal orientation of MAPbI3 films on PEDOT:PSS was examined using two-dimensional measurements. The results show that CHP films undergo some degree of crystallization, with the (110) planes predominantly orientated at an angle of 46° from the surface normal, perpendicular to a certain substrate. The CHP film without TA has the same preferred orientation as the CHP film, and it can be effectively coordinated between MAI and PbI2 to form self-assembled precursors.

The study focuses on the performance of photovoltaic devices in different scanning directions, with some results being better than others. CHP devices show the highest average performance and the narrowest distribution for all parameters among the fabrication methods. The volume ratio of CHP to DMF is critical for the formation of the CHP film. CBdrp devices have comparable performance parameters with CHP devices, but the distribution for parameters is broader than those of CHP devices. The study focuses on the performance of IFF devices compared to processed CHP and CBdrp devices, highlighting the challenges in controlling the quality of PbI2 and residual PbI2 resulting from fabrication conditions. The TRPL decay curves showed that the fast decay component might originate from the quenching of free carrier transport from MAPbI3 to PEDOT:PSS or PC61BM, while the slow decay component could come from radiative recombination. UPS measurements were performed to study the electronic properties of MAPbI3 films, which can be related to device performance depending on the fabrication method. The study suggests that IFF devices can be seriously affected by the combination of light and applied voltage, leading to low Jsc and high Voc, corresponding to a heavily n-doped sample with MAI-deficient films and poor device performance [29].

Conclusion

The study explores the impact of solution-processed MAPbI3 fabrication methods on planar perovskite solar cells based on PEDOT:PSS. It found that MAPbI3 with preferred orientation improves charge transfer and has low doping density. The processing method is more suitable for practical applications, while immersion methods are inappropriate. I-V hysteresis is dominant in all fabrication methods. The researchers need to find accurate measurement conditions and develop universally reproducible fabrication methods to compensate for intrinsic MAPbI3 properties. Acknowledging imperfections and presenting current research problems is crucial for better understanding and suggestions for new methods and records.

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Conflict of Interest Statement

The authors conducted ethical and transparent research, demonstrating the importance of ethical practices in scientific research.

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