engineering proceedings

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Proceeding Paper

Towards Manufacture Stable Lead Perovskite $APbI_3$ (A = Cs, MA, FA) Based Solar Cells with Low-Cost Techniques †

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† Presented at the 1st International Conference on Energy, Power and Environment, Gujrat, Pakistan, 11–12 November 2021.

Abstract: Herein, we examine the impact of cations on the structural, morphological, optical properties and degradation of lead perovskite $APbI_3$ (where A = MA, FA, Cs). Its structure, surface morphology and optical properties have been investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM) and UV-Visible spectrometer. The structure of perovskite thin films was found to be in the direction of (110) plane. It is seen from the XRD results that this kind of cation assumes a significant part in stabilising and improving the performance of APbI3 based solar cells. Here, the cesium lead iodide thin films show a smooth and homogenous surface and enormous grain size without pinhole perovskite film. An optical investigation uncovered that the band gap is in a range from 1.4 to 1.8 eV for the different cations. Additionally, in ~60% humidity under dark conditions for two weeks, the structural and optical properties of CsPbI3 films remained good. Furthermore, the efficiency of FTO/TIO2/CSPbI3/Spiro-Ometad/Au solar cells was calculated to be 21.48%.

Keywords: thin films; hybrid perovskite; optical properties; phase stability; efficiency

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Citation: Bouich, A.; Marí-Guaita, J.; Bouich, A.; Pradas, I.G.; Marí, B. Towards Manufacture Stable Lead Perovskite $APbI_3$ (A = Cs, MA, FA) Based Solar Cells with Low-Cost Techniques. *Eng. Proc.* **2021**, *12*, 81. https://doi.org/10.3390/engproc2021012081

Academic Editor: Shahid Iqbal

Published: 12 January 2022

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1. Introduction

Perovskites solar cells have shown a huge improvement in efficiency in recent years; with an increase in power conversion efficiency (PCE) of 3.8% in 2009 to more than 25% in 2019 [1]. Furthermore, due to the flexibility of Perovskites as a result of their incorporation with different elements, there still exists a window for further increase in PCE in the future [2]. In ABX_3 perovskite, A is the cation where A = (MA, FA, or Cs), B is a small cation where B = (Pb or Sn . . .) and X is the anion where X = (Cl, I or Br). Numerous techniques have been utilized for the manufacture of perovskite solar cells. Among them are the one-step spin coating technique [3] and the two-step spin coating technique, both techniques are easy to control and produce perovskite thin films [4]. Due to their optimal bandgap of about 1.47 eV for photovoltaic applications, Quantum Dot APbI3 lead iodide materials are considered suitable perovskite materials. However, they do have a problem regarding their stability [5]. Here, we show that cation A affects the morphological and optical properties of $APbI_3$, and investigate the stability of $CsPbI_3$, $FaPbI_3$, and $MaPbI_3$. Findings show that $CsPbI_3$ shows a stable structure under a relative humidity of ~60%.

2. Thin Films Preparation

All compounds, lead iodide (PbI2, 99%), formamidinium iodide (FAI), methylammonium iodide MAI, cesium iodide (CsI), Lead iodide (PbI_2, 99%), DMF, DMSO as solvents, and chlorobenzene as anti-solvent was purchased from Sigma Aldrich, St. Louis, MO, USA.

The APbI3 (a = Cs, Fa, Ma) perovskite thin films were elaborated on clean FTO glasses. The perovskite solutions were made from 1 M FAI, MAI, CsI, (1 M PbI_2) and were dissolved in DMF solution for two hours. The mixed solutions were kept on a hot plate at 60 °C for two hours in a glovebox, then 100 µL was spin-coated at 3000 rpm for 10 s and 1 mL chlorobenzene was dropped onto the wet APbI3 films at 4000 rpm for 50 s. Consequently, the as-prepared APbI3 were thermally annealed at 120 °C for 10 min.

Thin films FAPbI3, MaPbI3, CsPbI3 structure were characterized by X-ray diffraction (XRD). Morphology images were taken by scanning electron microscope (SEM). Optical properties were performed using Ocean Optics HR4000 spectrophotometer and the performance was calculated by Scaps.

3. Results

The XRD analysis was examined for $FAPbI_3$, $MaPbI_3$, $CsPbI_3$ fresh and aged samples in Figure 1a–c, respectively. The aged $FAPbI_3$ shows degradation issues after two weeks and appears the non-perovskite δ-$FAPbI_3$ phase. This is verified by the augmentation of the peak characteristic of the δ phase, located at 12.6°. In the case of the sample $CsPbI_3$ aged, no additional peaks were shown, compared to the aged $MAPbI_3$, which demonstrated a dissociation of film into PbI_2.

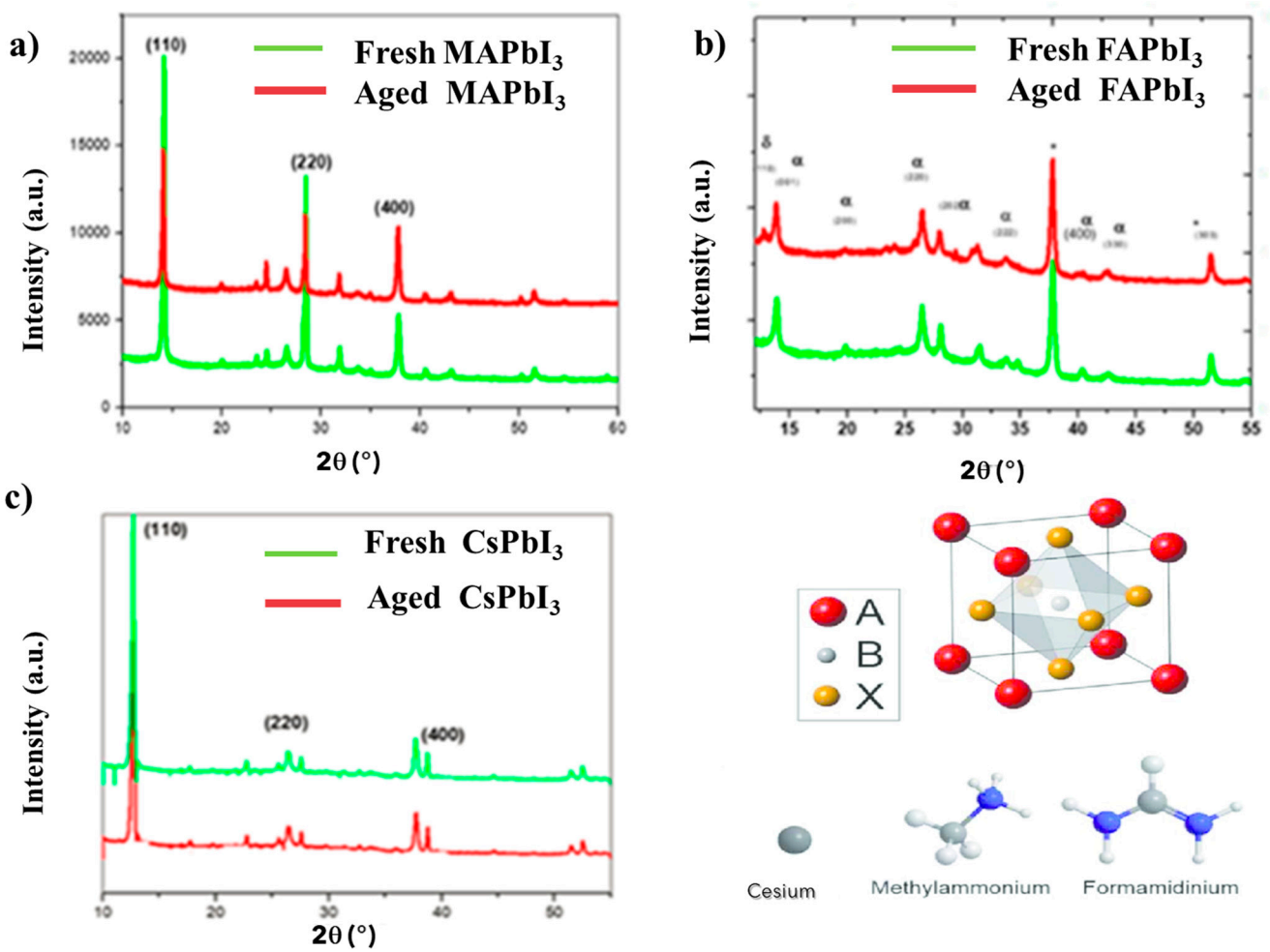

Figure 1. XRD pattern of fresh and aged samples of (**a**) $MaPbI_3$, (**b**) $FaPbI_3$ and (**c**) $CsPbI_3$.

Figure 2 displays SEM images of $MaPbI_3$, $FaPbI_3$ and $CsPbI_3$ fresh and aged that display the apparition of numerous pinholes and transformations in surface morphology compared to the Fresh $MAPbI_3$ and Fresh $FAPbI_3$, as we can note that for the $CsPbI_3$ surface,

less pinholes are seen after two weeks in humidity, which is in good agreement with the results of XRD that approve the stability of the $CsPbI_3$ sample.

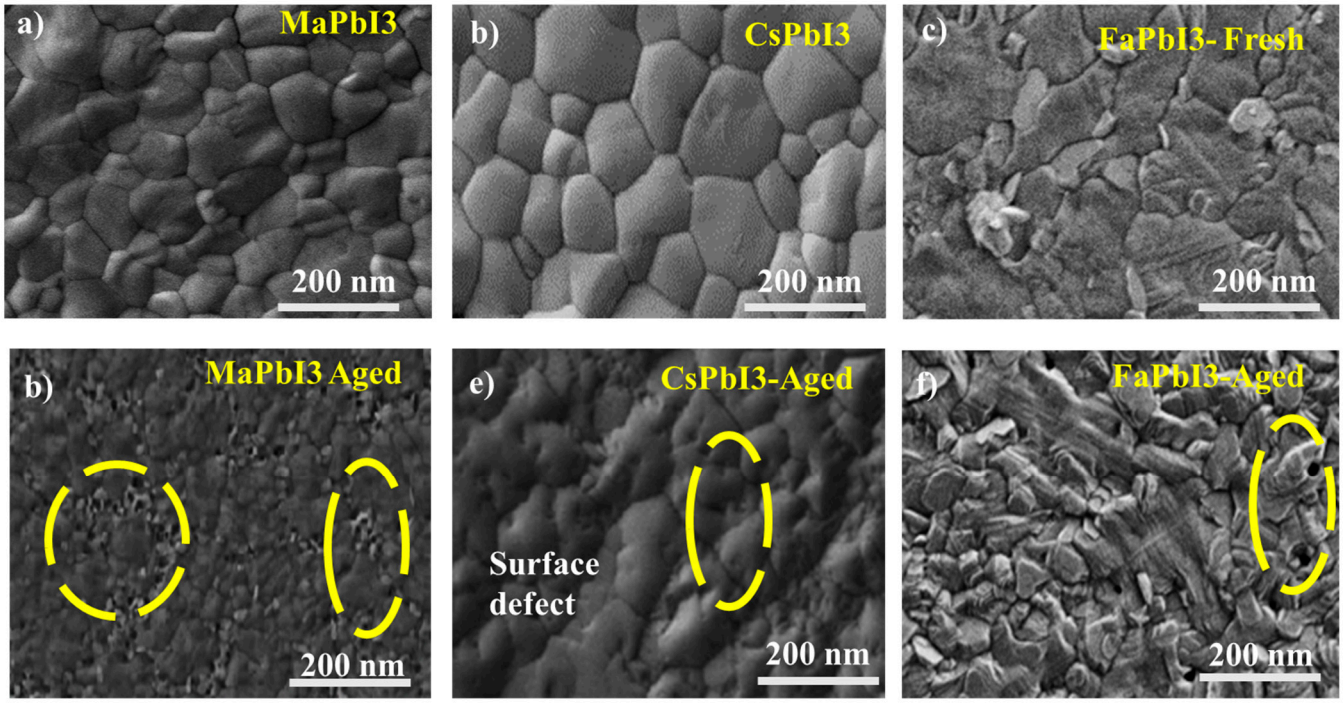

Figure 2. SEM images of $APbI_3$ where A = (Ma/ Fa/Cs) (**a**) Fresh $MaPbI_3$ Film (**b**) Fresh $FaPbI_3$ Film (**c**) Fresh $CsPbI_3$ Film (**d**) Aged $MaPbI_3$ Film (**e**) Aged $CsPbI_3$ Film (**f**) Aged $FaPbI_3$ Film.

XRD results correlate with the UV-visible measurements, which show a good bandgap [6] (Figure 3). A slow decrease in the absorption of aged $CsPbI_3$ intensity demonstrates the slow degradation of CsPbI3. Hence, our results suggest that cesium can slow the degradation of the perovskite structure of APbI3 films.

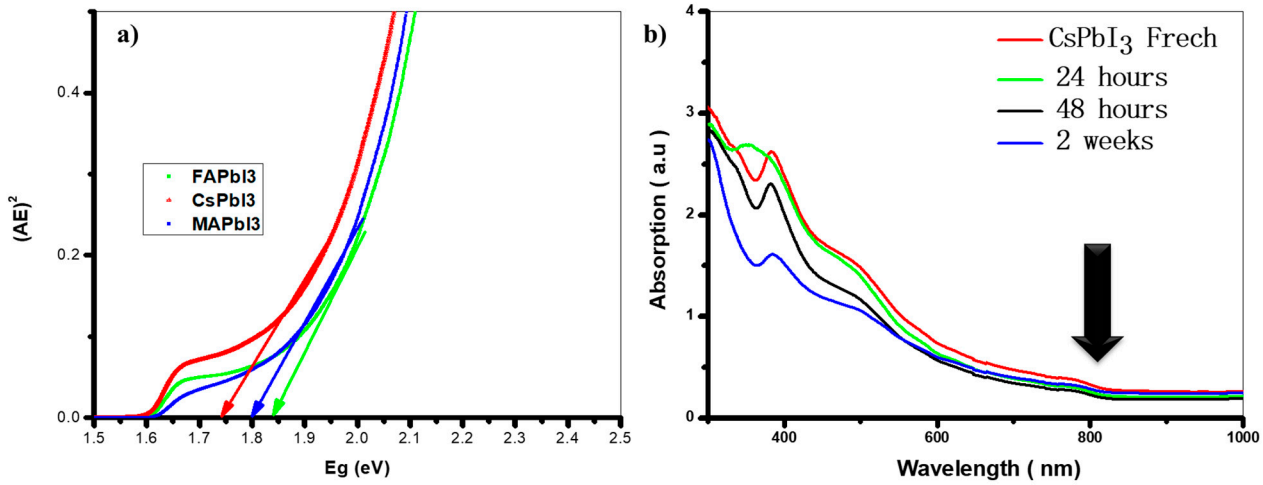

Figure 3. (**a**) Bandgap of $APbI_3$ where A = Cs, FA, MA, (**b**) the absorption of $CsPbI_3$ aged.

4. Performance of FTO/TiO_2/APbI3/Spiro-Ometad/Au

The performance FTO/TiO_2/APbI3/Spiro-Ometad/Au of solar cells where FTO is the back contact [7] through changes in the bandgap, SCAPS-1D software was used. The simulation parameters of $APbI_3$ were taken from our previous calculations, where the bandgap varied from 1.7 to 1.8 eV. Figure 4 shows the J-V characteristic curve; the P-V

curve shows that the maximum power is for $FaPbI_3$ and $CsPbI_3$. On the other hand, $CsPbI_3$ demonstrates the stable performance of solar cells (Table 1).

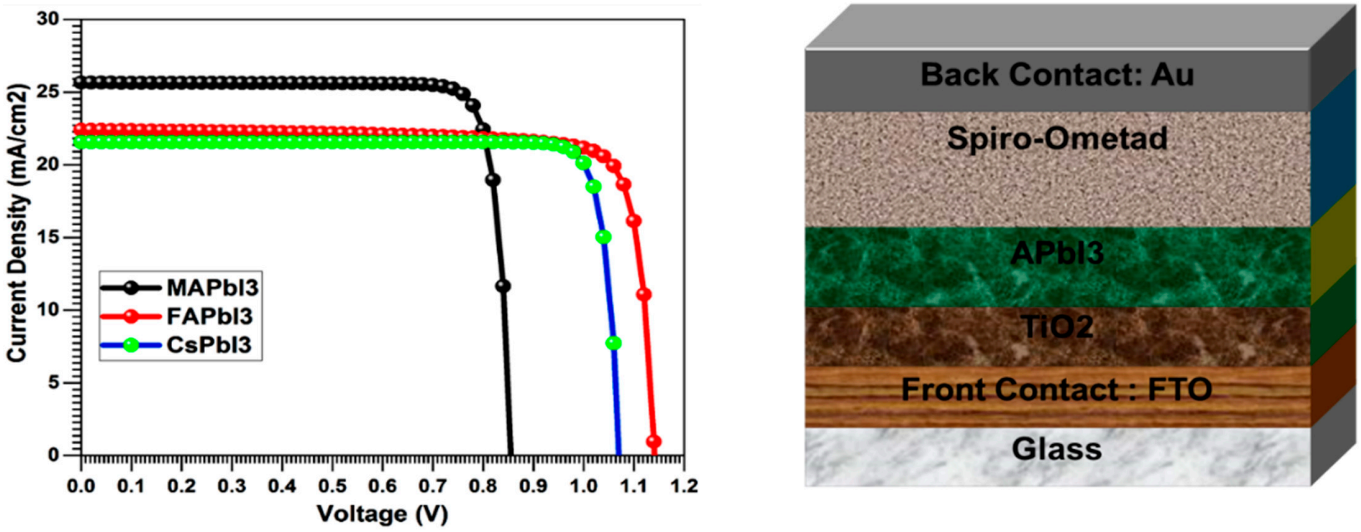

Figure 4. Performance of APbI3 (A = Cs, Fa, Ma) based solar cells.

Table 1. Characteristics of APbI3 (A = Cs, Fa, Ma) based solar cells.

Solar Cell	Voc	Jsc	FF	eta
	V	mA/cm^2	%	%
$MAPbI_3$	0.8562	25.654019	86.09	18.91
$FAPbI_3$	1.1413	22.401144	83.79	21.42
$CsPbI_3$	1.0715	21.571401	88.63	21.48

5. Conclusions

In this work, APbI3 perovskite thin films were determined using the spin-coating technique and the impact of cations on their stability and performance was investigated.

According to the results reported above, cesium may be the best option for the better performance of the cell, as it shows greater crystallinity and stability in humid conditions.

Author Contributions: Conceptualization, A.B. (Amal Bouich); methodology, A.B. (Amal Bouich); validation, B.M.; formal analysis, J.M.-G.; investigation, A.B. (Asmaa Bouich) and A.B. (Amal Bouich); resources, J.M.-G.; data curation, A.B. (Amal Bouich); writing—original draft preparation, J.M.-G.; writing—review and editing, A.B. (Amal Bouich), I.G.P. and B.M.; visualization, J.M.-G. and A.B. (Amal Bouich); supervision, B.M.; project administration, B.M.; funding acquisition, B.M. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by Ministerio de Economía y Competitividad (Spain), grant number PID2019-107137RB-C21.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Not applicable.

Acknowledgments: We would like to thank Ministerio de Economía y Competitividad (Spain) for supporting this work. the Author Amal Bouich acknowledged the post-doctoral contract supported by the RRHH.

Conflicts of Interest: The authors declare no conflict of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript, or in the decision to publish the results.

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