JNPV 2021 Abstract submission (Poster)
7 -Cellules hybrides et organiques, pérovskites

Interface design of perovskite solar cells: application of molecular additives to improve the stability and the performance

Claire DARIN BAPAUME[1], Mathieu FREGNAUX[2], Thomas VINCENT[3], Muriel BOUTTEMY[2], Philip SCHULZ[1]

1. Centre nationale de la recherche scientifique (CNRS), UMR9006 Institut Photovoltaïque d'Ile de France (IPVF) Joint unit research– 18 boulevard Thomas Gobert, 91120 Palaiseau
2. Institut Lavoisier de Versailles (ILV), Université de Versailles Saint-Quentin-en-Yvelines, Université Paris-Saclay, CNRS, UMR 8180, 45 avenue des Etats-Unis, 78035 Versailles Cedex, France
3. Institut Photovoltaïque d'Ile de France (IPVF) – 18 boulevard Thomas Gobert, 91120 Palaiseau

Few years after its first conception, perovskite solar cells (PSC) had shown a great evolution from the dye-sensitized device with organic halide perovskite (HaP) by Kojima et al at 3.8%[1] in 2009 to organic-inorganic halide triple cation perovskite device, reaching now 25.5% of power conversion efficiency (PCE). The interface design of PSCs is a key point to control and optimize in order to develop a stable device with higher power conversion efficiency[2,3]. Plenty of publications present interface engineering by adding a layer between the charge transport layer and the perovskite[4–8]. The objective of this interlayer is twofold: improve the photovoltaic performance but also the stability of the cell. In our case, I am working mainly on the hole transport layer / HaP interface (top interface in n-i-p configuration) based on the organic compound adamantane, $C_{10}H_{16}$, and its derivatives[9]. Adamantane (AD) and its derivatives are "bulky" hydrophobic molecules, likely to behave as a protection layer to prevent humidity to degrade the absorber. Using optoelectrical characterization and XPS analysis (fig.1), the additives' effects on the device and the perovskite layer are identified. Using the application of the molecular film (fig.2), we observe a moderate improvement of the open-circuit voltage (Voc) and the fill factor (FF). Furthermore, we performed stability tests of unencapsulated devices incorporating these additives in ambient atmosphere and under illumination for 70 hours. 1-adamantanamine hydrochloride (1ADAHCl) is showcased to be the most promising additive by preserving 56% of its initial PCE compared to 22% for the reference sample without adamantane-base interlayer.

Figure 1

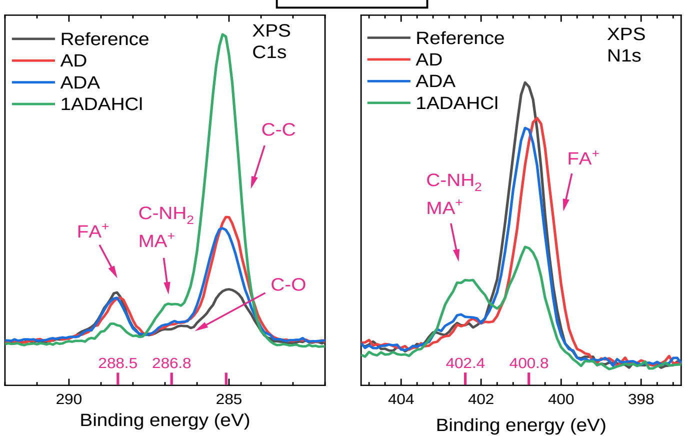
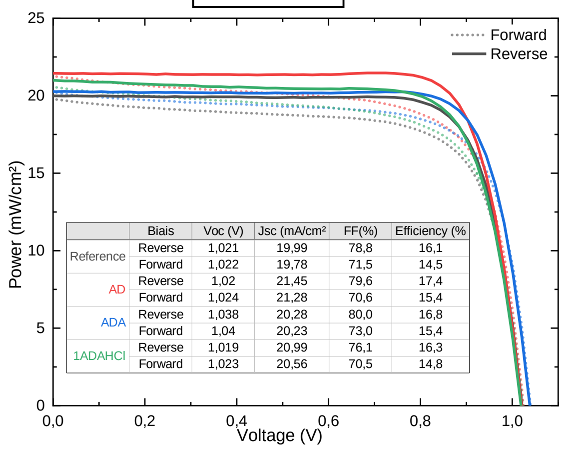


Figure 2



	Biais	Voc (V)	Jsc (mA/cm²	FF(%)	Efficiency (%
Reference	Reverse	1,021	19,99	78,8	16,1
	Forward	1,022	19,78	71,5	14,5
AD	Reverse	1,02	21,45	79,6	17,4
	Forward	1,024	21,28	70,6	15,4
ADA	Reverse	1,038	20,28	80,0	16,8
	Forward	1,04	20,23	73,0	15,4
1ADAHCl	Reverse	1,019	20,99	76,1	16,3
	Forward	1,023	20,56	70,5	14,8

1. Kojima, A., Teshima, K., Shirai, Y. & Miyasaka, T. Organometal halide perovskites as visible-light sensitizers for photovoltaic cells. *J. Am. Chem. Soc.* **131**, 6050–6051 (2009).
2. Schulz, P., Cahen, D. & Kahn, A. Halide Perovskites: Is It All about the Interfaces? *Chem. Rev.* **119**, 3349–3417 (2019).
3. Aydin, E., De Bastiani, M. & De Wolf, S. Defect and Contact Passivation for Perovskite Solar Cells. *Adv. Mater.* **31**, 1–20 (2019).
4. Su, H. *et al.* The Application of Graphene Derivatives in Perovskite Solar Cells. *Small Methods* **4**, 1–12 (2020).
5. Magomedov, A. *et al.* Self-Assembled Hole Transporting Monolayer for Highly Efficient Perovskite Solar Cells. *Adv. Energy Mater.* **8**, (2018).
6. Wol, C. M. *et al.* Perfluorinated Self-Assembled Monolayers Enhance the Stability and Efficiency of Inverted Perovskite Solar Cells. **15**, (2020).
7. Cells, L. P. S. *et al.* Polymer/Inorganic Hole Transport Layer for Low-Temperature-Processed Perovskite Solar Cells. *Energies* **13**, 1–12 (2020).
8. Kegelmann, L. *et al.* It Takes Two to Tango - Double-Layer Selective Contacts in Perovskite Solar Cells for Improved Device Performance and Reduced Hysteresis. *ACS Appl. Mater. Interfaces* **9**, 17245–17255 (2017).
9. Tavakoli, M. M. *et al.* Adamantanes Enhance the Photovoltaic Performance and Operational Stability of Perovskite Solar Cells by Effective Mitigation of Interfacial Defect States. *Adv. Energy Mater.* **8**, 1–7 (2018).