Tailor-made amino-based Self-assembled monolayer grafted on an electron transport ZnO layer; Perovskite solar cells performance and modified interface relationship

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Reference : *ACS Applied Energy Materials* **2022** *5* (2), 1635-1645
DOI: 10.1021/acsaem.1c03050
DOI : https://10.1021/acsaem.1c03050
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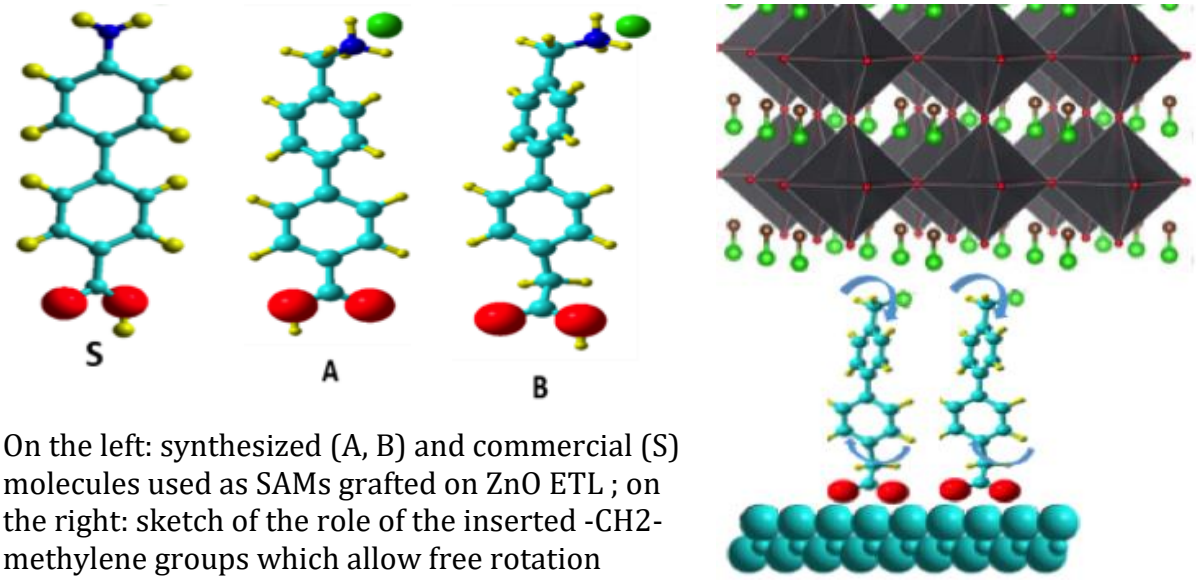
Abstract :
Self-assembled monolayer (SAMs) have been grafted via a carboxylic acid function onto a ZnO electron transport layer to control the growth and structure of a hybrid perovskite $CH_3NH_3PbI_3$ (MAPI) used as the active layer in a solar cell. In addition of the basic molecule, HO_2C-PP-NH_2 (PP = biphenyl), two bipolar molecules, HO_2C-$(CH_2)_n$-PP-CH_2-NH_3Cl (A: n = 0), 4'-(carboxy)-(1,1'-biphenyl)-4-aminomethyl hydrochloride, and B: (n = 1), 4'-(carboxymethyl-(1,1'-biphenyl)-4-aminomethyl hydrochloride, are used in this work. They have been tailored in order to ensure (i) rigidity/self-assembly and conductivity via the biphenyl and (ii) some flexibility via the methylene groups, to ensure bonding both to the solid ZnO layer and to the methylammonium lead Iodide (MAPI) layer. The protonated amino group was chosen to create an efficient 2D sub-layer for the growth of the methylammonium-based perovskite. The deposition of SAMs on the metal oxide layers improves device stability and the efficiency of perovskite solar cells (PCSs). The SAMs enhance the long-term stability of PSCs in ambient air atmosphere.



On the left: synthesized (A, B) and commercial (S) molecules used as SAMs grafted on ZnO ETL ; on the right: sketch of the role of the inserted -CH2- methylene groups which allow free rotation around the C-NH2 and C-COO single bonds and therefore which increase the structural compatibility between the MAPI, "biphenyl" and ZnO lattices