

Molecular tuning in self-assembled molecules for applications as selective contacts in optoelectronic devices

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Self-assembled molecules (SAMs) are low molecular weight organic molecules that can form ordered arrays onto a substrate of few nanometers thick, when using an adequate bonding group. Moreover, molecular engineering of the SAMs can lead to ordered unidirectional ultrathin functionalized films. Currently, SAMs are widely applied in the architecture of optoelectronic devices due to their ease of synthesis and processing. Their good performance as charge extracting layers, mainly as hole selective contact, have contributed to the increase in efficiency and stability in both lead and tin-based perovskite solar cells (PSCs).[1,2] The structure of the SAMs can be divided in three distinct sections: i) the anchoring group, usually made by carboxylic or phosphonic acids, that forms covalent bonds with metal oxides, ii) the linker, that determine the packing geometry, and iii) the functional groups, that interact with the photoactive layer and, thus, have a crucial influence on the interfacial effects. The fine tuning of the different components modulates the efficiency and stability the optoelectronic properties by, for example, modifying the work function of the ITO electrode or the morphology of the layer deposited on top.

Therefore, careful design of the groups forming part of the SAMs will have different effects on the performance of the devices. For example, the addition of a second phenyl moiety in the linker increases the luminance and light emission lifetime in perovskite-based light emitting diodes because of a twofold effect. [3] On one hand, the variation of the thickness of the emissive layer, and on the other, the increased electron delocalization that favors the extended lifetime emission. Similarly, in PSCs, the incorporation of different moieties on the functional groups will have different effects on the charge kinetics, that will be reflected in the power conversion efficiency of the devices.[4]

References

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