

Abstract Submitted
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Engineering **hybrid**
polymer/metal-oxide interfaces by self-assembled molecular interlayers

ALESSANDRO MATTONI, mattoni@iom.cnr.it — Hybrid organic heterojunctions are of great technological interest as both optically active layers as well as hole blocking interfaces in organic or hybrid solar cells. Despite the potential of combining processable organic polymers with inorganic components, they have not yet demonstrated high efficiencies. A promising approach towards more efficient systems consists in engineering the interface by self-assembled molecular interlayers that can selectively affect the interactions of the donor and acceptor components. A combination of molecular dynamics and electronic structure calculations [1] we study thermodynamic and optoelectronic properties of polymer/metaloxide interfaces in presence of several molecular interlayers such as metal-organic macrocyclic complexes [2,4] or pyridine derivatives [1]. The theoretical results are tested on specifically designed hybrid solar cells providing evidence of impressive enhancement of interface properties.

- [1] M. I. Saba, et al. *J. Phys. Chem. C* 115, 9651–9655 (2011).
- [2] C. Melis et al. *ACS Nano* 5 9639 (2011).
- [3] E. Canesi et al., *Energy Environ. Sci.* 5 9068 (2012).
- [4] G. Mattioli et al. Submitted (2013)/

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