Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Photoexcited Charge-Transfer Separation at Donor-Acceptor Organic Interfaces: Molecular Configuration and Surface Functionalization Effects

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I. DENSITY FUNCTIONAL HYBRID CALCULATIONS FOR C_{60} AND ZNPC INTERFACES

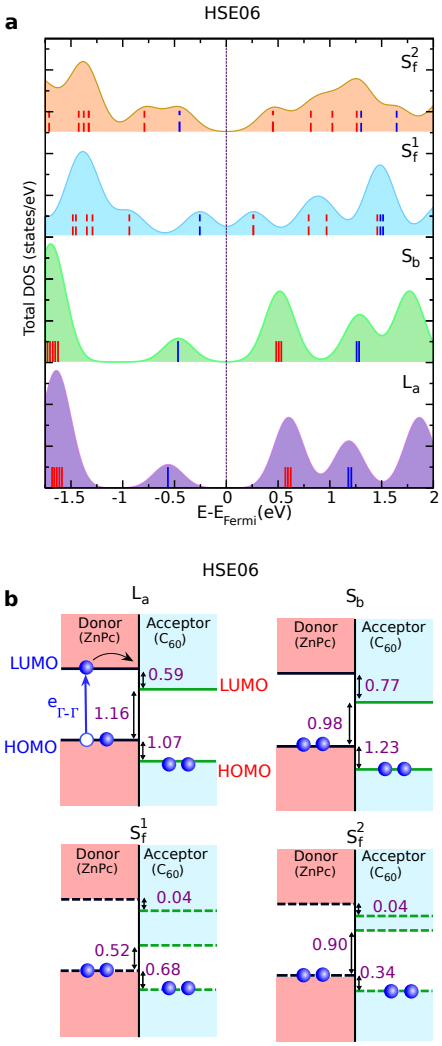

FIG. 1S: Hybrid HSE06 calculations for L_a, S_b, S_f^1 and S_f^2 configurations. **a**, Calculated total density of states (states/eV) as a function of energy (eV). For clarity, curves have been shifted and smoothed with a Lorentzian broadening of 0.200 eV. The major contributions of each molecule, that is C_{60} and ZnPc, on each interface around the Fermi level is marked by the vertical bars in blue and red colors. The Fermi level is set to zero. **b**, Energy level diagrams (eV) showing the main states involved in the photo-excitation dynamics at the Donor (ZnPc) and Acceptor (C_{60}) heterointerfaces similarly to Figure 1 in the main text.

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