Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Enhanced Conductivity and Photoresponse in Rubrene Single-Crystal/PCBM Film Heterojunctions

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SUPPORTING INFORMATION

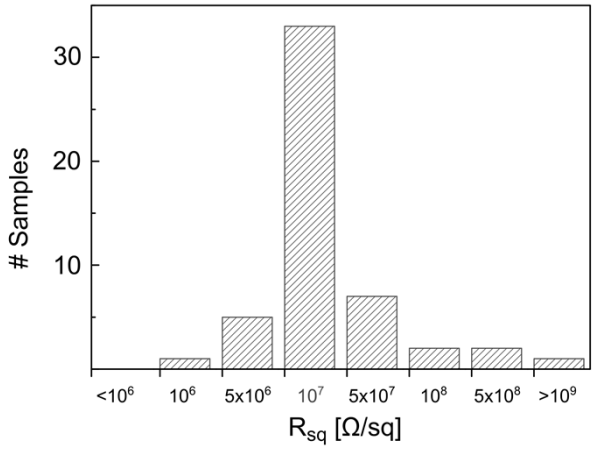

Figure S1. Histogram of the sheet resistance values of PCBM/rubrene interfaces, in a two-probe configuration for 50 samples.

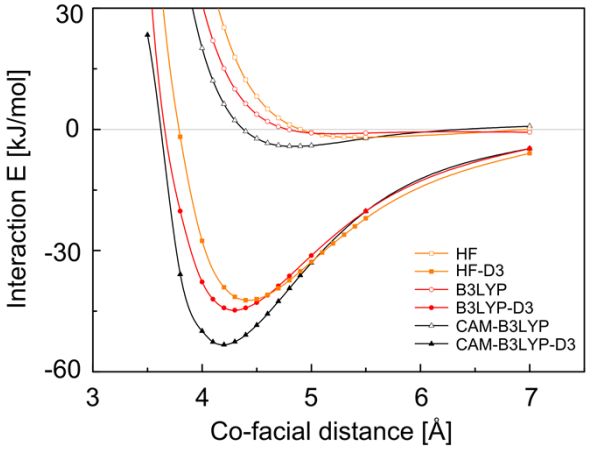

Figure S2. Evolution of the interaction energy of PCBM/rubrene with co-facial approximation, computed with HF and DFT B3LYP, including dispersion energy (-D3) and long-range corrections (CAM-).

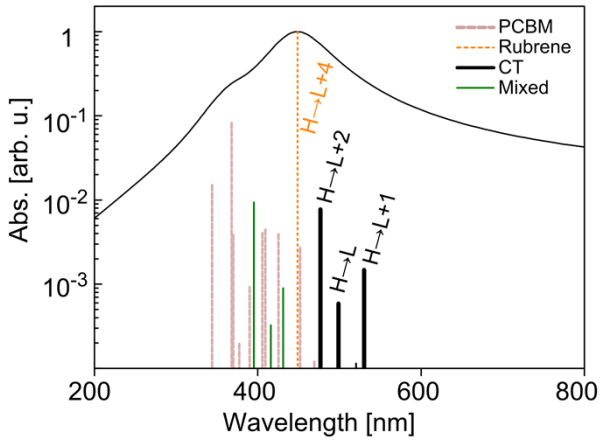

Figure S3. Absorption stick spectrum of the interface (z=4.2 Å), showing the degree of delocalization of singlet excitations, from TD-DFT results obtained at the CAM-B3LYP/6-31G level of theory.

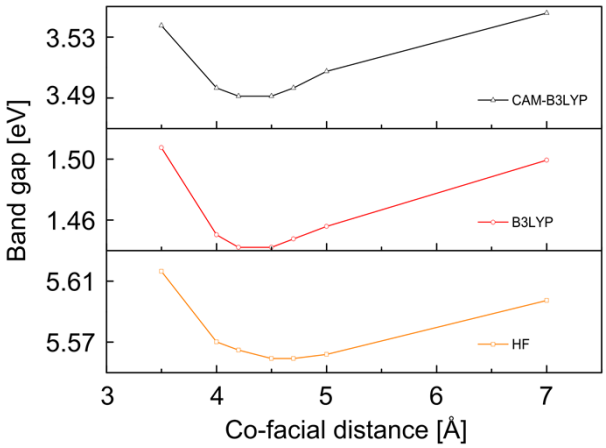

Figure S4. Evolution of the band gap with PCBM/rubrene distance, in co-facial approximation, computed at different levels of theory.

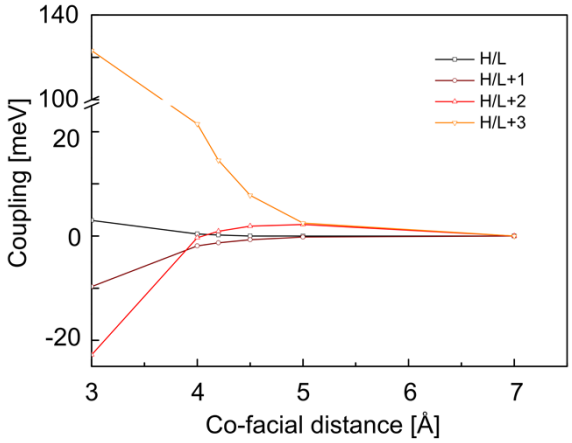

Figure S5. Effective electronic coupling between HOMO (rubrene) and LUMO to LUMO+3 (PCBM), as a function of co-facial approximation, evaluated using the projective method on CAM-B3LYP results.

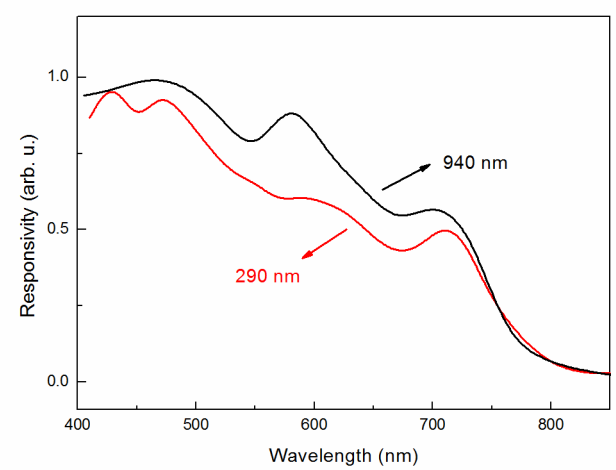

Figure S6. Normalized responsivity of PCBM/rubrene interfaces, using rubrene crystals of different thicknesses (290 and 940 nm) on top of PCBM films (~500 nm).

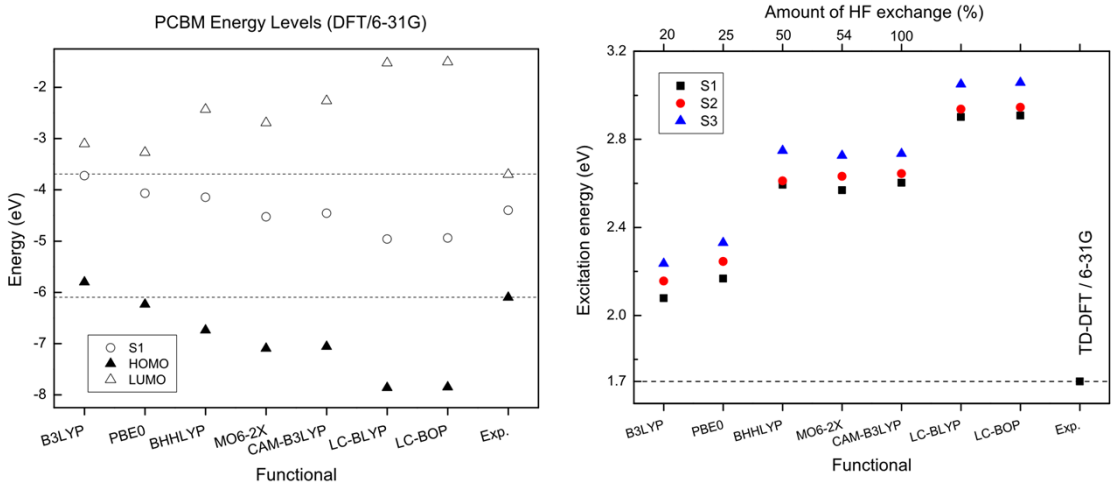

Figure S7. DFT functional pre-screening based for PCBM, using HOMO, LUMO and singlet excitation energies as figures of merit.

Table S1. Computed and experimental ionization energies (IE), electron affinities (EA) and electronic bandgaps, for rubrene and PCBM, in eV. Theoretical IE and EA are estimated via Koopmans' theorem.

	Rubrene SC [1, 2]			**PCBM film [3]**		
	IE	EA	Electronic bandgap	IE	EA	Electronic bandgap
Exp.	4.85	2.05	2.80	6.1	3.7	2.4
HF	6.13	1.02	5.11	7.55	0.50	7.05
B3LYP	4.63	1.92	2.71	5.80	3.10	2.70
CAM-B3LYP	5.83	0.99	4.84	7.06	2.26	4.80

[1] N. Sai et al, Phys. Rev. B, 2008, 77, 161306.
[2] Y. Nakayama et al, Appl. Phys. Lett., 2008, 93, 173305.
[3] E. J. Meijer et al, Nat. Mater., 2003, 2, 678.