Supporting Information

Description of the Charge Transfer States at the Pentacene/C_{60} Interface: Combining Range-Separated Hybrid Functionals with the Polarizable Continuum Model

Zilong Zheng,[1] Jean-Luc Brédas,[2*] and Veaceslav Coropceanu[1*]

[1] *School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics*

Georgia Institute of Technology, Atlanta, Georgia 30332-0400

[2] *Solar & Photovoltaics Engineering Research Center,*

Division of Physical Science and Engineering,

King Abdullah University of Science and Technology,

Thuwal 23955-6900, Saudi Arabia

[*]E-mails: jean-luc.bredas@kaust.edu.sa; coropceanu@gatech.edu

Table S1. Energies (in eV) of the HOMO, LUMO, IP, and EA of pentacene, C_{60}, and the pentacene/C_{60} complex, using the optimally tuned BNL/6-31G(d,p) functional

		ω(vac)	ω(PCM)/PCM
PEN	HOMO	-6.10	-4.66
	IP	-6.11	-4.67
	LUMO	-0.94	-1.93
	EA	-0.95	-1.93
C_{60}	HOMO	-7.60	-5.69
	IP	-7.59	-5.70
	LUMO	-1.82	-2.68
	EA	-1.81	-2.70
P/C_{60}	HOMO	-5.82	-4.45
	IP	-5.82	-4.50
	LUMO	-2.34	-2.98
	EA	-2.33	-3.02

Table S2. Energies (in eV) of the HOMO, LUMO, IP and EA of pentacene, C_{60}, and the pentacene/C_{60} complex, using the optimally tuned ωB97XD/6-31G(d,p) functional.

		ω(vac)	ω(vac)/PCM	ω(PCM)/PCM
PEN	HOMO	-6.10	-6.15	-4.88
	IP	-6.09	-5.12	-4.87
	LUMO	-1.00	-1.05	-1.97
	EA	-1.01	-2.07	-1.99
C_{60}	HOMO	-7.71	-7.62	-6.24
	IP	-7.69	-6.68	-6.24
	LUMO	-1.91	-1.82	-2.81
	EA	-1.91	-2.73	-2.81
P/C_{60}	HOMO	-5.96	-6.04	-4.83
	IP	-5.97	-5.08	-4.84
	LUMO	-2.07	-1.95	-2.86
	EA	-2.03	-2.06	-2.84

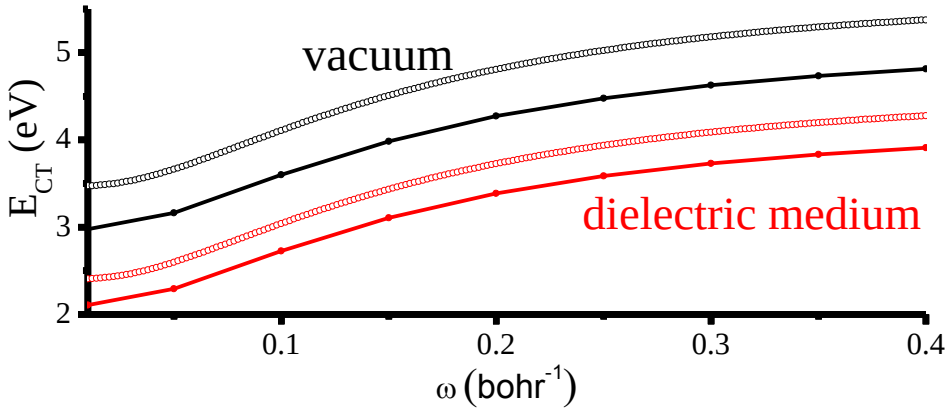

Figure S1. Dependence of the energy of the lowest CT state of the pentacene/C_{60} complex as a function of the RS parameter obtained by means of constrained DFT (CDFT) in vacuo (black line) and in a ε=3 dielectric medium (red line); open circles and solid circles correspond, to 1.0 and 0.9 Becke charge transferred from donor to acceptor, respectively.