Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Table S1. The energies (eV) of the CdSe bands, HOMO/LUMO of the anchored phthalocyanine molecule and HOMO of the phenylbutyric linker, calculated using BAND code with different exchange-correlation functionals.

	PBEsol		BLYP		LDA	
Tilting angle	*ca.* 80º	*ca.* 30º	*ca.* 80º	*ca.* 30º	*ca.* 80º	*ca.* 30º
VBM	-5.91	-5.88	-5.55	-5.53	-6.10	-6.06
CBM	-4.42	-4.35	-4.06	-4.00	-4.71	-4.64
Linker	-5.71	-5.70	-5.42	-5.43	-5.96	-5.90
PC-HOMO	-5.03	-5.15	-4.72	-4.83	-5.25	-5.38
PC-LUMO	-3.63	-3.77	-3.34	-3.46	-3.86	-4.00

Table S2. The energies (eV) of the CdSe bands, HOMO/LUMO of the anchored phthalocyanine molecule and HOMO of the phenylbutyric linker, calculated using BAND code with PBEsol functional and different basis sets.

	DZ		TZP		TZ2P	
Tilting angle	*ca.* 80º	*ca.* 30º	*ca.* 80º	*ca.* 30º	*ca.* 80º	*ca.* 30º
VBM	-6.21	-6.15	-5.91	-5.88	-5.88	-5.85
CBM	-4.75	-4.64	-4.42	-4.35	-4.40	-4.34
Linker	-6.05	-6.06	-5.71	-5.70	-5.74	-5.73
PC-HOMO	-5.54	-5.71	-5.03	-5.15	-5.05	-5.17
PC-LUMO	-4.10	-4.29	-3.63	-3.77	-3.64	-3.75

Table S3. The energies (eV) of the CdSe bands, HOMO/LUMO of the anchored phthalocyanine molecule and HOMO of the phenylbutyric linker, calculated using plane-wave approach implemented in VASP code with different exchange-correlation functionals. The cutoff energy was 700 eV. We used a 3×1×3 Monkhorst-Pack grid for the k-point sampling in LDA and GGA PBEsol calculations and a gamma point in PBE0 calculations.

	PBEsol		PBE0		LDA	
Tilting angle	*ca.* 80º	*ca.* 30º	*ca.* 80º	*ca.* 30º	*ca.* 80º	*ca.* 30º
VBM	-3.53	-3.50	-4.26	-4.33	-3.68	-3.64
CBM	-2.45	-2.40	-1.63	-1.68	-2.68	-2.63
Linker	-3.44	-3.45	-4.24	-4.31	-3.62	-3.60
PC-HOMO	-2.78	-2.89	-3.28	-3.41	-2.95	-3.06
PC-LUMO	-1.56	-1.69	-0.97	-1.12	-1.71	-1.86