

Improving optoelectronic and charge transport properties of D- π -D type diketopyrrolopyrrole-pyrene derivatives as multifunctional materials for organic solar cells applications

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Table S1 Calculated the longest absorption wavelengths λ_{abs} of parent molecule **1** in chloroform by various methods with 6-31G(d,p) basis set, along with available experimental data.

Methods	λ_{abs}
B3LYP/6-31G(d,p)	615
PBE0/6-31G(d,p)	583
CAM-B3LYP/6-31G(d,p)	503
LC- ω PBE/6-31G(d,p)	452
ω B97XD /6-31G(d,p)	493
M062X /6-31G(d,p)	507
Exp ^[a]	589

^[a] Experimental results of **1** were taken from Ref. [39].

Table S2 The Calculated E_{HOMO} and E_{LUMO} (in eV) for PC₆₁BM and PC₇₁BM at PBE0/6-31G (d,p) and B3LYP/6-31G (d,p) levels, along with available experimental data.

Methods	PC ₆₁ BM		PC ₇₁ BM	
	E_{HOMO}	E_{LUMO}	E_{HOMO}	E_{LUMO}
PBE0/6-31G (d,p)	-5.98	-3.99	-5.92	-3.82
B3LYP/6-31G (d,p)	-5.67	-3.75	-5.61	-3.60
EXP ^[a]	-6.00	-3.80	-6.00	-3.95

^[a] Experimental results of PC₆₁BM and PC₇₁BM were taken from Refs [52] and[53], respectively.

Table S3 The differences between the E_{HOMO} of **1–8** and the E_{LUMO} of PC₆₁BM and PC₇₁BM ($\Delta E_{\text{L-H}}$) at the PBE0/6-31G(d,p) level.

Molecules	$\Delta E_{\text{L-H}}^{[\text{a}]}$	$\Delta E_{\text{L-H}}^{[\text{b}]}$
1	1.12	1.29
2	1.34	1.51
3	1.07	1.24
4	1.19	1.36
5	1.24	1.41
6	1.28	1.45
7	1.20	1.37
8	1.40	1.57

^[a] $\Delta E_{\text{L-H}}$ values for PC₆₁BM as acceptor; ^[b] $\Delta E_{\text{L-H}}$ values for PC₇₁BM as acceptor.