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Journal Name

ARTICLE

Supporting Information

Highly Efficient Emitters of Ultra-Deep-Blue Light Made from Chrysene Chromophores

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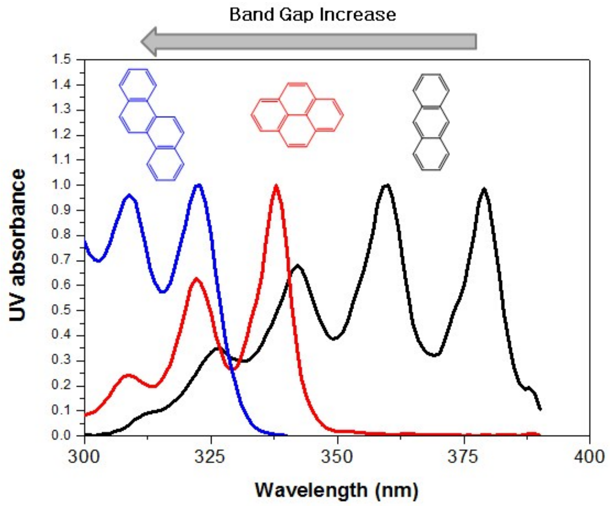

Fig S1. UV-vis absorption normalized spectra of anthracene, pyrene and chrysene in solution state.

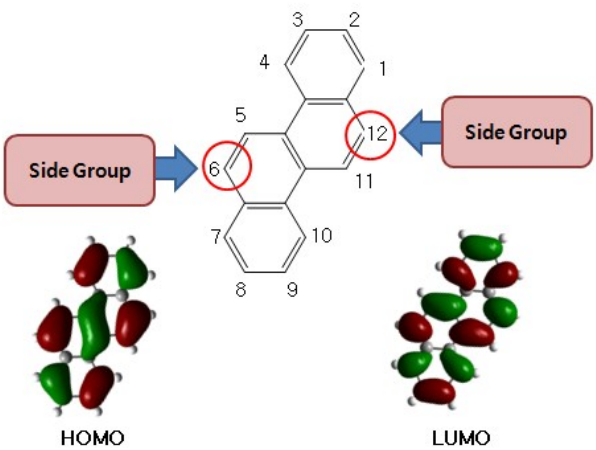

Fig S2. Electron density distribution of chrysene chromophore.

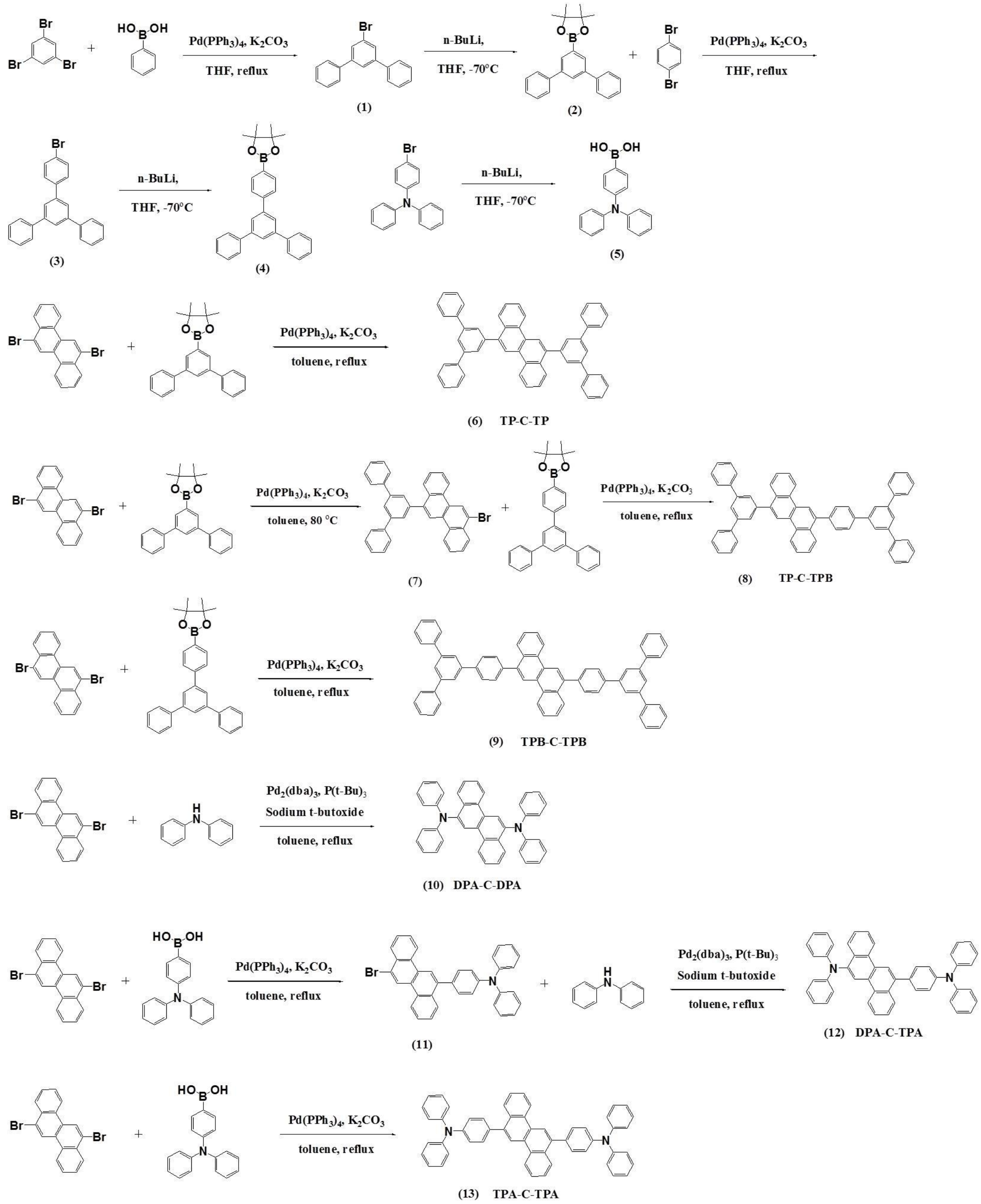

Fig S3. Synthetic routes of chrysene derivatives.

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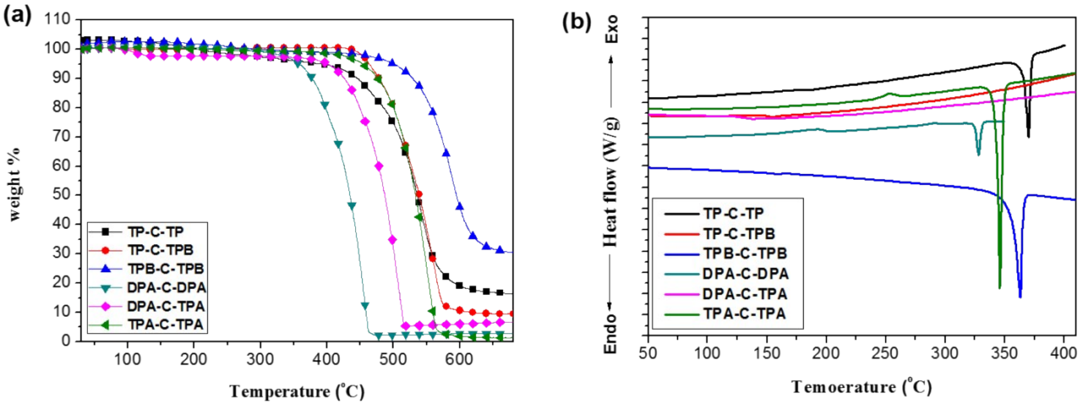


Fig S4. Thermal properties of chrysene derivatives. (a) TGA curves, (b) DSC curves.

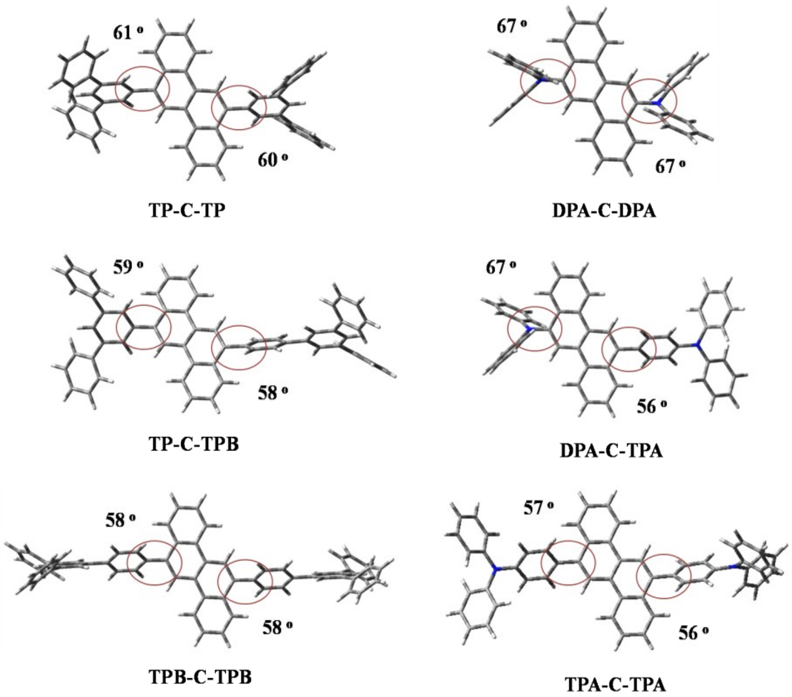


Fig S5. Dihedral angles of the S_0 states of the compounds calculated at the CAM-B3LYP/6-311G (d,p) level.

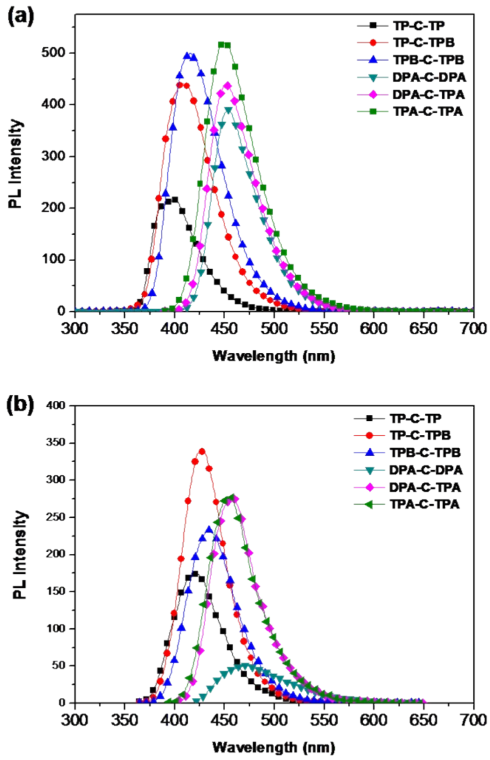


Fig S6. PL spectra of chrysene derivatives: (a) solution state, (b) film state.

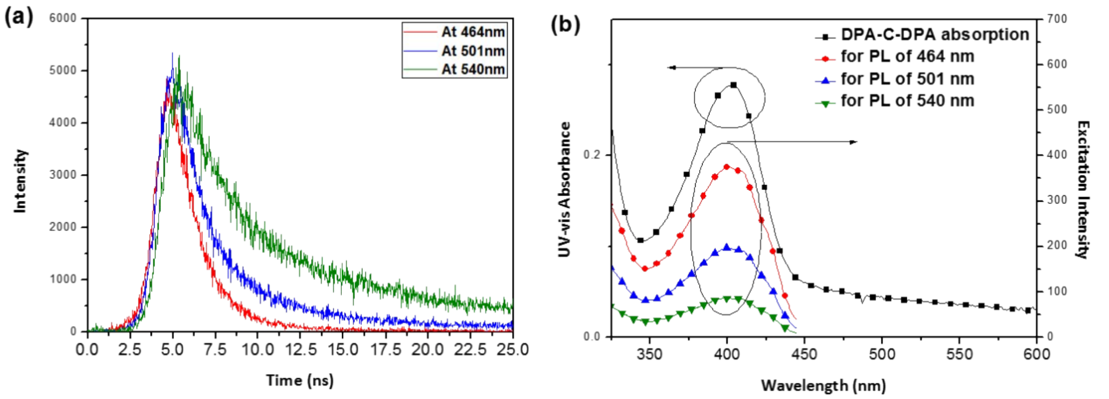


Fig S7. (a) Time-resolved emission decays, (b) UV-vis absorption spectrum and excitation spectra of DPA-C-DPA film (thickness: 100nm).

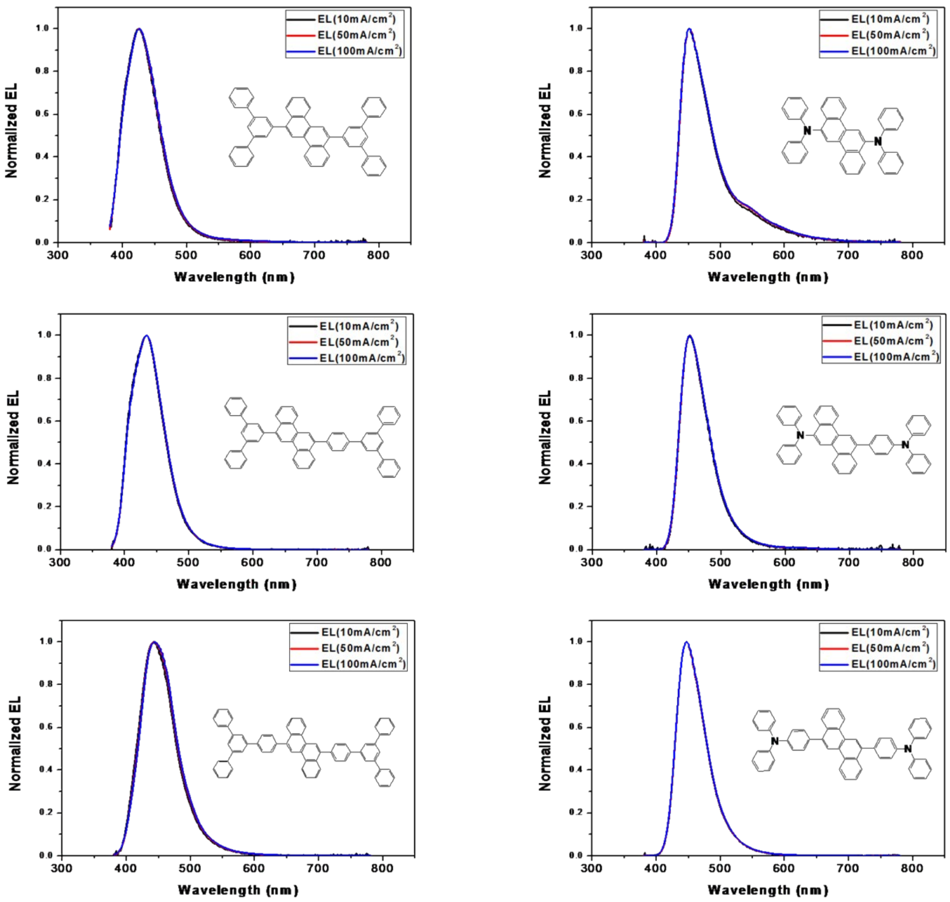
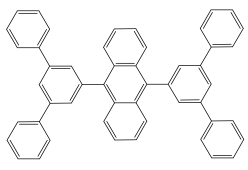
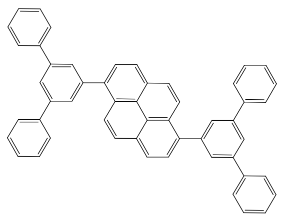


Fig S8. Normalized EL spectra of synthesized compounds.

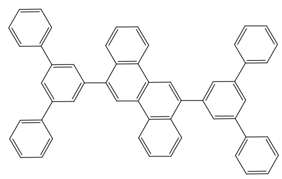
Table S1. Optical properties of anthracene, pyrene and chrysene core compounds.



MAM



TP-Py-TP



TP-C-TP

Compounds	Solution[(a)] UV (nm)	Solution[(a)] PL (nm)	Solution[(a)] FWHM (nm)	Film[(b)] UV (nm)	Film[(b)] PL (nm)	Film[(b)] FWHM (nm)	PL QY[c] (%)	HOMO (-eV)	LUMO (-eV)	Band gap (eV)
MAM	377, 398	433	53	383, 402	439	62	39	6.01	3.05	2.96
TP-Py-TP	365	411	51	372	460	80	67	5.99	2.90	3.09
TP-C-TP	279, 337	400	52	279, 342	417	59	35	5.88	2.64	3.24

(a) 1x 10^{-5} M in chloroform, (b) Film thickness: 50nm on the glass, (c) The solid-state absolute quantum yield on the quartz plate using an integrating sphere apparatus.

Table S2. Absorption energies and oscillator strengths calculated using TD-CAM-B3LYP/6-311G(d,p) for synthesized compounds.

Compounds	λ_{abs} (nm)	$\lambda_{emission}$ (nm)	Oscillator Strength(f)	Characteristic of Transition	Contribution (%)
TP-C-TP	307	397	0.48	HOMO-1→LUMO HOMO-1→LUMO+1 HOMO → LUMO HOMO → LUMO+1	5.7 2.8 73.5 5.6
TP-C-TPB	309	406	0.71	HOMO-1→LUMO HOMO-1→LUMO+1 HOMO→LUMO HOMO→LUMO+1	2.8 2.7 80.5 3.3
TPB-C-TPB	312	412	0.99	HOMO-1→LUMO+1 HOMO→LUMO	3.6 85.2
DPA-C-DPA	349	426	0.51	HOMO-1→LUMO+2 HOMO→LUMO	2.3 90.1
DPA-C-TPA	338	423	0.69	HOMO-1→LUMO HOMO-1→LUMO+2 HOMO→LUMO	12.9 2.0 73.9
TPA-C-TPA	321	422	1.27	HOMO-2→LUMO HOMO→LUMO	22.7 60.5

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