Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Elucidating π-π Interaction-Induced Extension Effect in Sandwich Phthalocyaninato Compounds

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Caption of Content

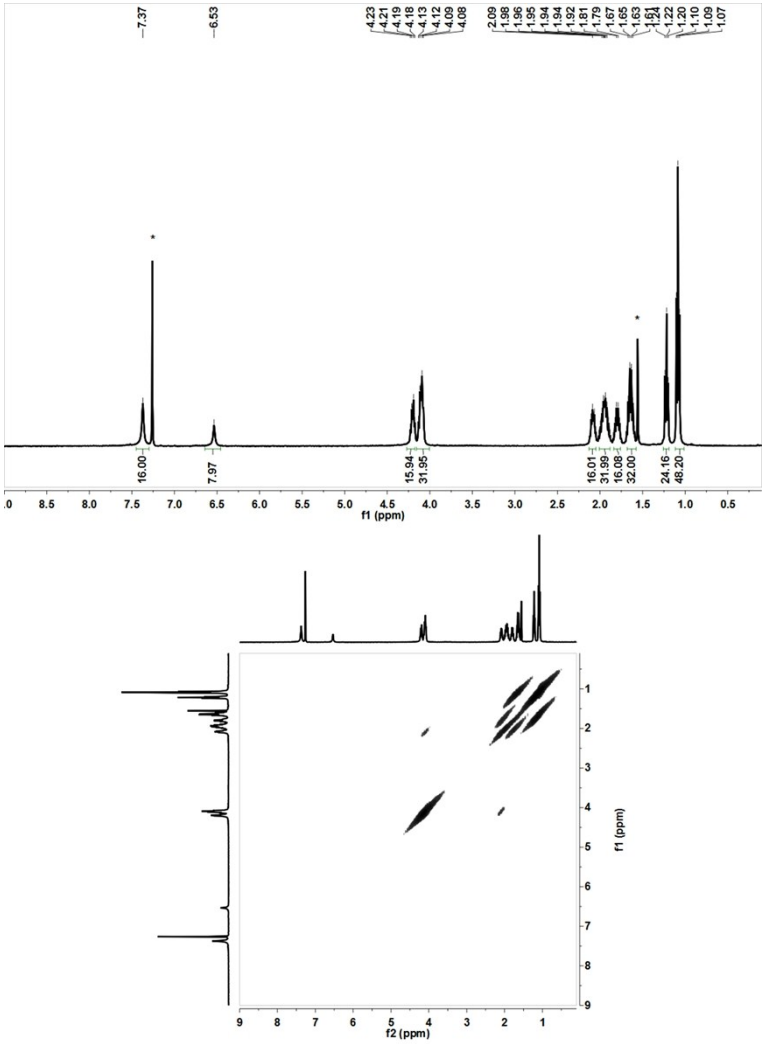

Fig S1. ^{1}H NMR and ^{1}H-^{1}H COSY spectra of **3** in $CDCl_3$

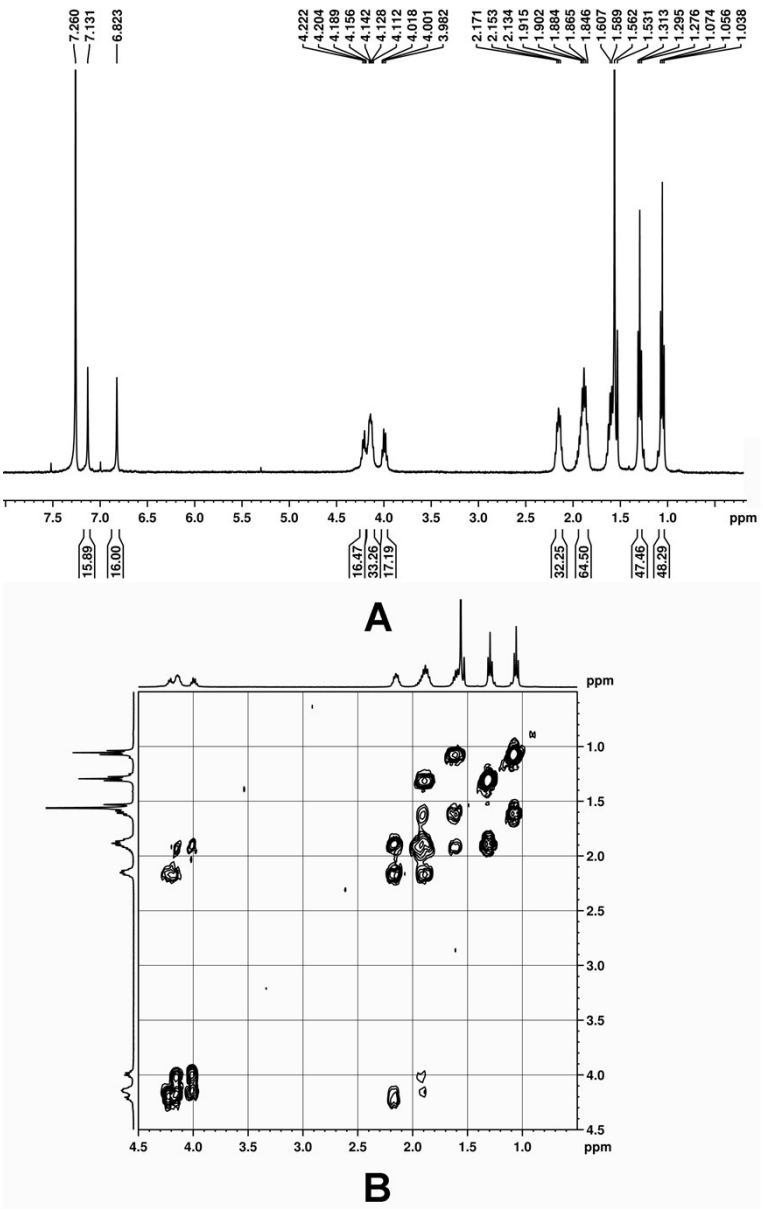

Fig S2. ^{1}H NMR and ^{1}H-^{1}H COSY spectra of **4** in $CDCl_3$.

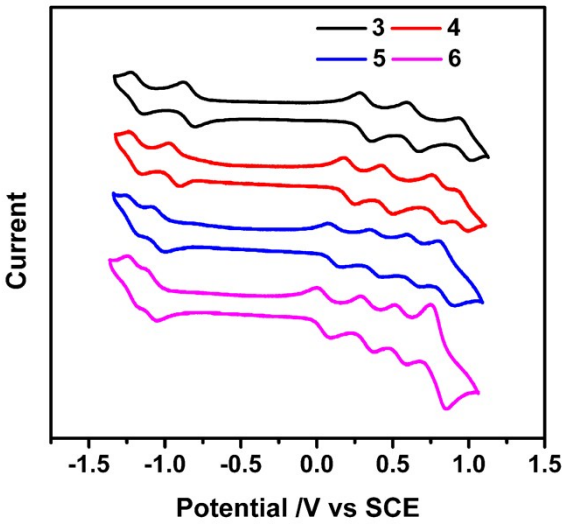

Fig S3. Cyclic voltammetry of quintuple-decker complexes {[(Pc*)Sm][(Pc*)Cd_n(Pc*)$_n$][Sm(Pc*)]} (n = 0-3) (**3**-**6**) in CH_2Cl_2 containing 0.1 M [NBu_4][ClO_4] at the scan rate of 40 mV/s.

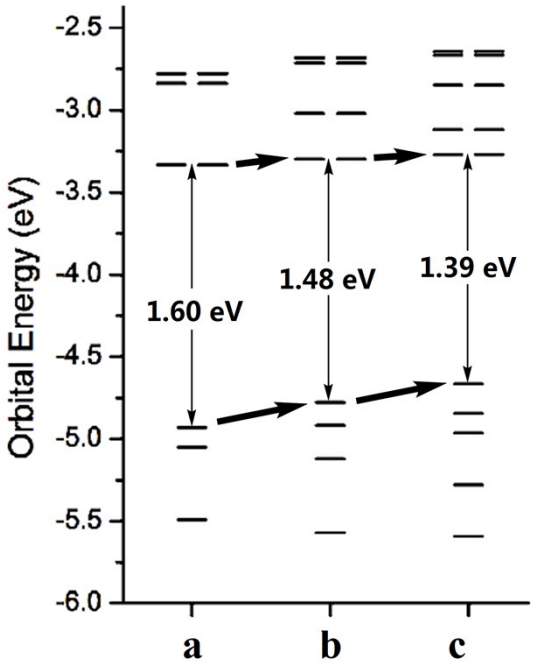

Fig S4. The frontier molecular orbital energies for {[(Pc)La][(Pc)Cd_n(Pc)$_n$][La(Pc)]} (n = 0-2) (**a**-**c**).

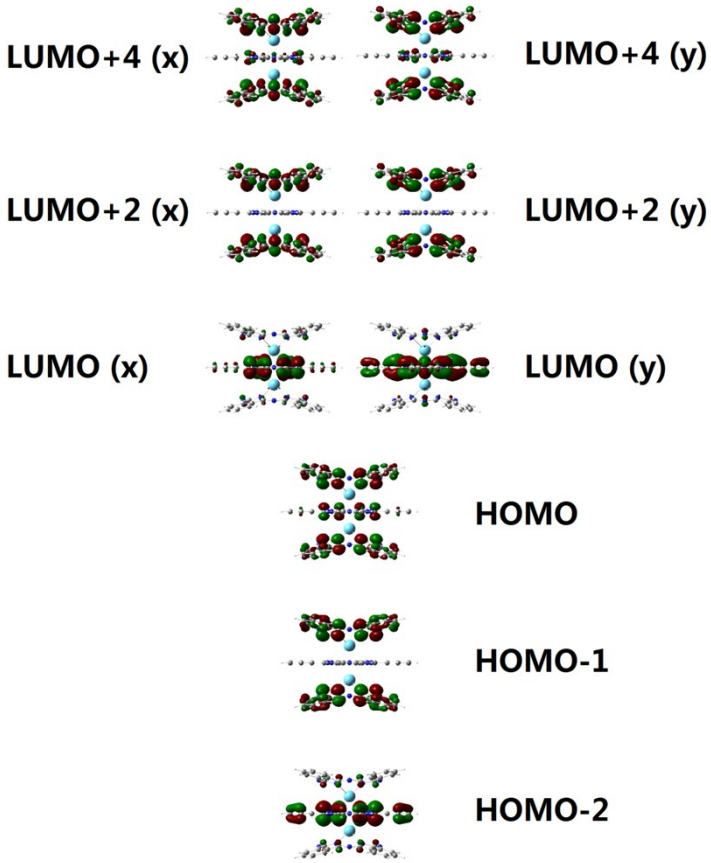

Fig S5. Frontier molecular orbital map for (Pc)La(Pc)La(Pc).

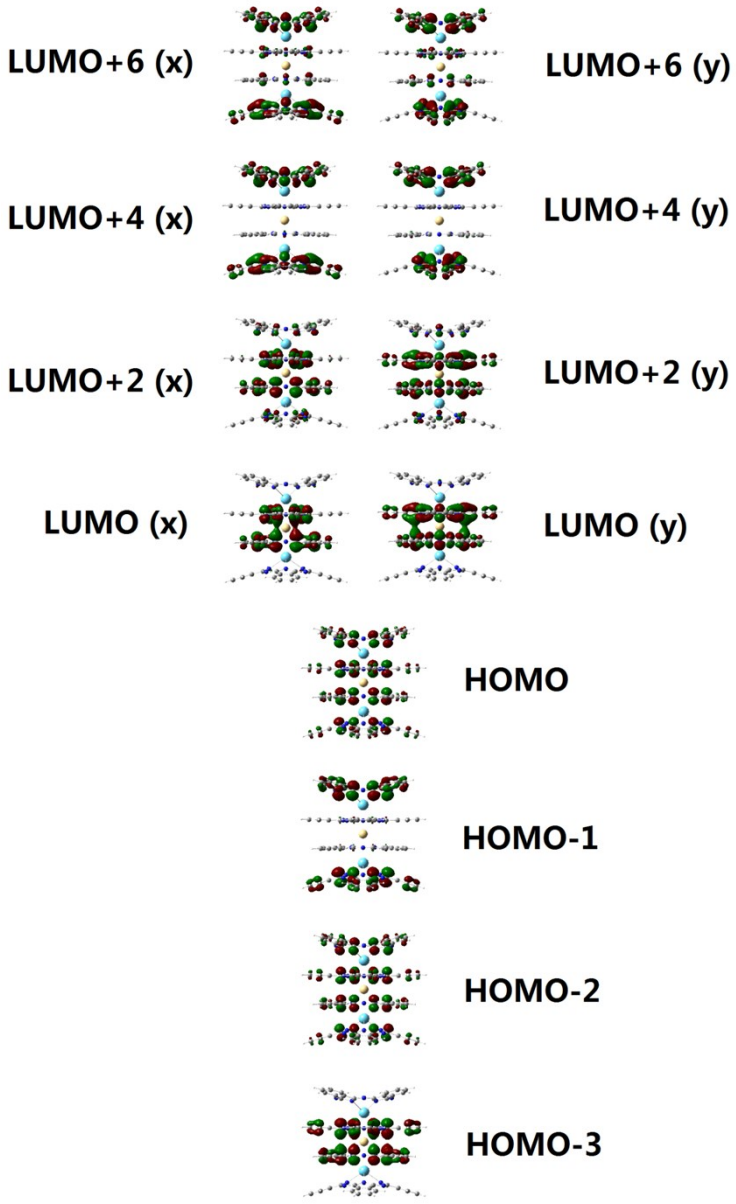

Fig S6. Frontier molecular orbital map for (Pc)La(Pc)Cd(Pc)La(Pc).

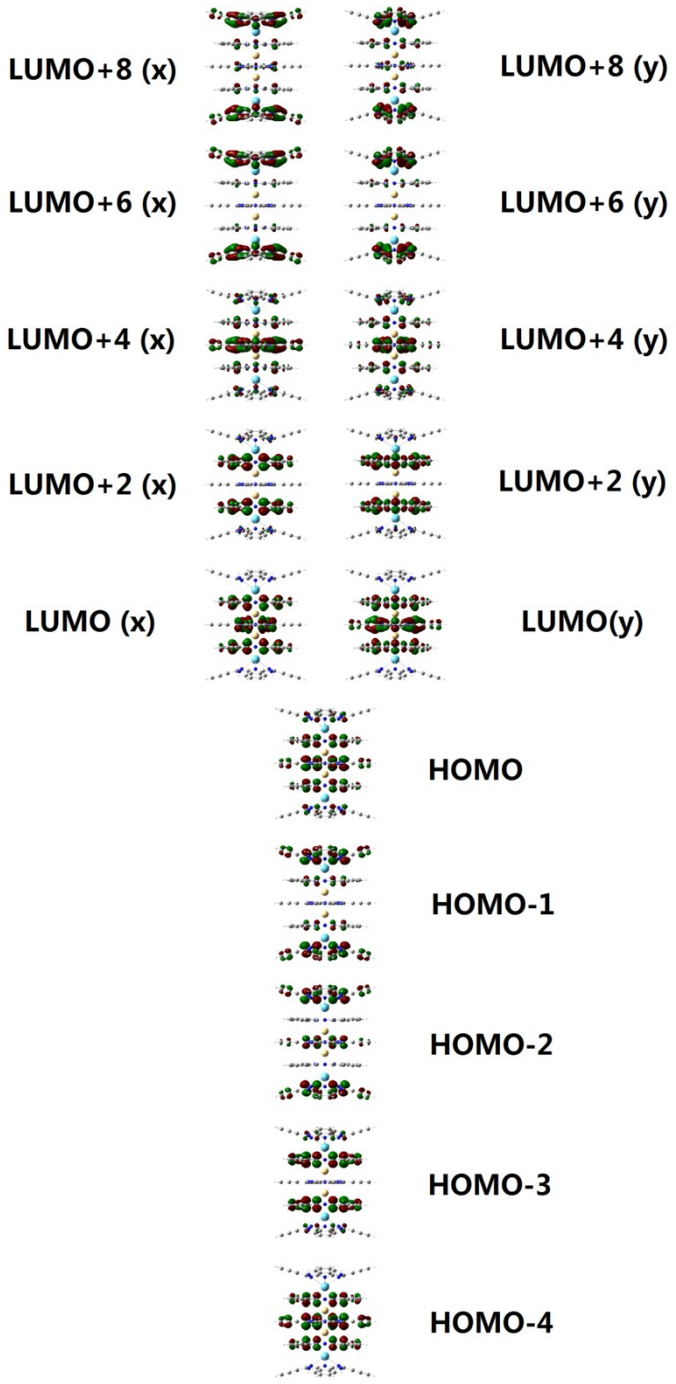

Fig S7. Frontier molecular orbital map for (Pc)La(Pc)Cd(Pc)Cd(Pc)La(Pc).

Table S1. Half-wave redox potentials of the compounds **3**-**6**.[a]

Compound	$\mathbf{Oxd_4}$	$\mathbf{Oxd_3}$	$\mathbf{Oxd_2}$	$\mathbf{Oxd_1}$	$\mathbf{Red_1}$	$\mathbf{Red_2}$	$\mathbf{\Delta E^o_{1/2}}$
3	--	0.98	0.63	0.33	-0.85	-1.18	1.18
4	0.94	0.79	0.47	0.22	-0.95	-1.20	1.17
5	0.85	0.64	0.39	0.12	-1.05	-1.22	1.17
6	0.81	0.55	0.34	0.06	-1.09	-1.22	1.15

[a] Recorded with $[Bu_4N][ClO_4]$ as electrolyte in CH_2Cl_2 (0.1 mol dm^{-3}) at ambient temperature. Potentials were obtained by cyclic voltammetry with a scan rate of 40 mV s^{-1}, and are expressed as half-wave potentials ($E_{1/2}$) in V relative to SCE unless otherwise stated.