Supporting Information

Effects of Benzo-Annelation of Asymmetric Phthalocyanine on the Photovolatic Performance of Dye-Sensitized Solar Cells

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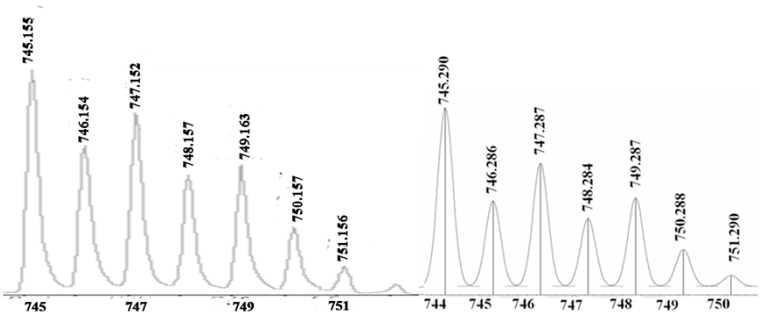

Fig. S1. Experimental (left) and simulated (right) isotopic pattern for the molecular ion of Zn-*tri*-TAPNc (a) shown in the MALDI-TOF mass spectrum.

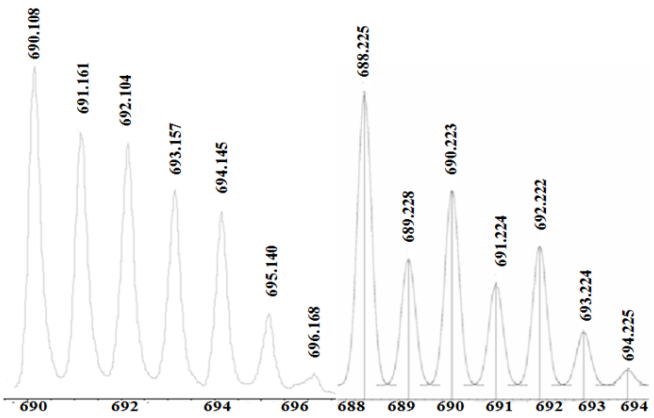

Fig. S2. Experimental (left) and simulated (right) isotopic pattern for the molecular ion of Zn-*tri*-TAPNc shown in the MALDI-TOF mass spectrum.

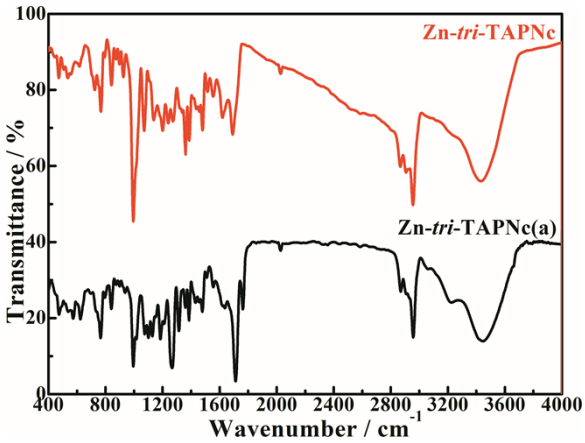

Fig. S3. IR spectra of Zn-*tri*-TAPNc (a) and Zn-tri-TAPNc.

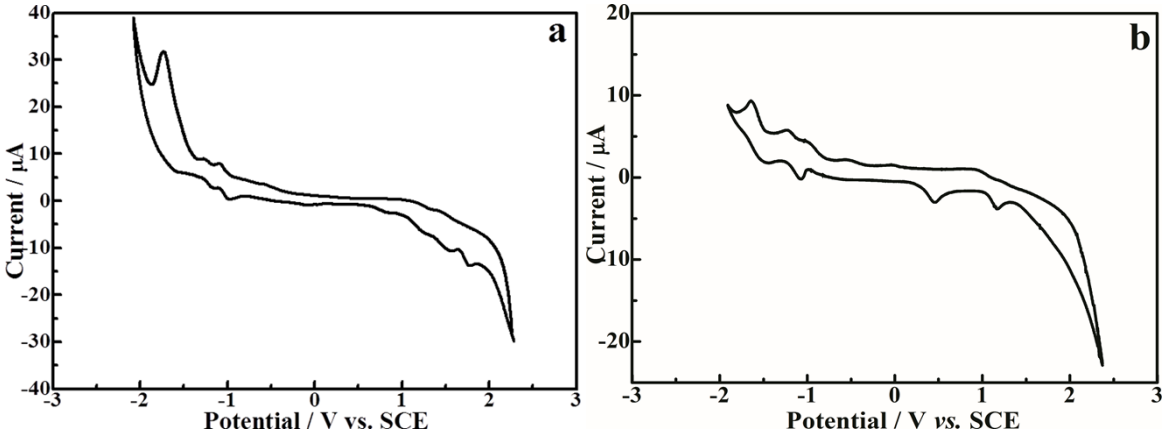

Fig. S4. The typical cyclic voltammograms of Zn-*tri*-TAPNc (a) and Zn-*tri*-PcNc (b) [1] in DCB containing 0.1 M $[NBu_4][ClO_4]$ at a scan rate of 20 $mV \cdot S^{-1}$.

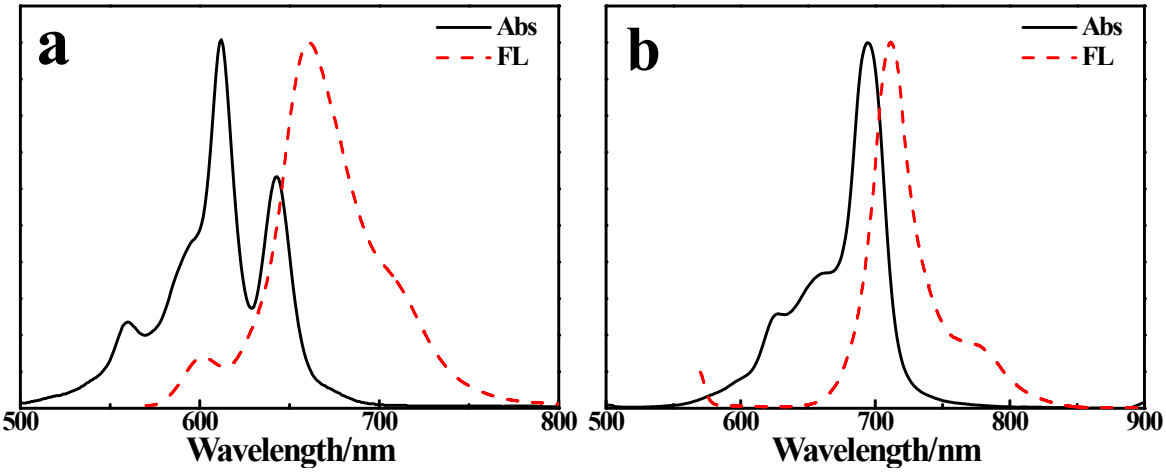

Fig. S5. The absorption and emission spectra of the asymmetrical Zn-*tri*-TAPNc (a) and Zn-*tri*-PcNc (b) in EtOH solution.

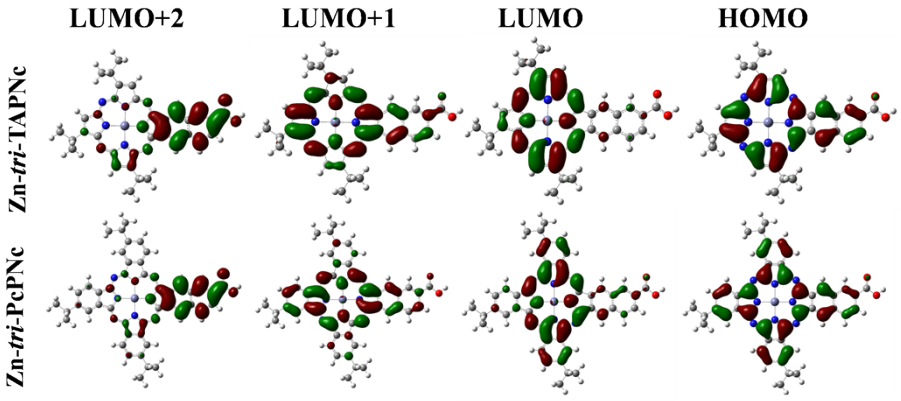

Fig. S6. The frontier molecular orbitals of the asymmetrical Zn-*tri*-TAPNc and Zn-*tri*-PcNc, full optimized at B3LYP/6-31G level.

Table S1. Electrochemical data of Zn-*tri*-TAPNc and Zn-*tri*-PcNc.

Dye	Oxd_2	Oxd_1	Red_1	Red_2	Red_3	$\Delta E^o_{1/2}$[a]
Zn-*tri*-TAPNc	1.15	0.75	-1.03	-1.21	-1.63	1.78
Zn-*tri*-PcNc	1.08	0.36	-1.13	-1.54	-1.91	1.49

[a] $\Delta E^o_{1/2}$ is the potential difference between the first oxidation and first reduction processes, i.e. the HOMO-LUMO gap of corresponding molecule.