

# Electronic supplementary information (ESI<sup>†</sup>)

## Synthesis, electron transports, and charge storage properties of fullerene–zinc porphyrin hybrid nanodiscs

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## Experimental methods

### Synthesis of H<sub>2</sub>TANP

Anhydrous dichloromethane (40 ml) was taken in a 100 ml round bottom flask under nitrogen atmosphere. To this dichloromethane solvent freshly distilled pyrrole (144 $\mu$ l, 2.08 mmol) and 5-acenaphthene carboxaldehyde (380 mg, 2.08 mmol) was added. After few minutes TFA (220 mg, 1.93 mmol) was added to this reaction mixture. The reaction mixture was then stirred for another 2 h at inert atmosphere. Finally DDQ (1.16 g, 5.1 mmol) was added to this mixture and it was stirred for 3 h in open air. Final purification was done by using a silica gel column. The yield was 90 mg (19%). Anal. Calcd (found) for C<sub>68</sub>H<sub>46</sub>N<sub>4</sub> (H<sub>2</sub>TANP): C, 88.86 (88.95); H, 5.04 (5.14); N, 6.10 (5.91). UV-Vis (dichloromethane):  $\lambda_{\text{max}}/\text{nm}$  ( $\epsilon/\text{M}^{-1}\text{cm}^{-1}$ ): 427(343000), 517(22940), 552(7490), 590(6761), 647(2699). <sup>1</sup>H NMR (400 MHz, CHLOROFORM-*d*)  $\delta$  – 2.29 (s, 2 H), 3.66-3.71 (m, 16 H), 6.85 - 7.01 (m, 4 H), 7.11 - 7.19 (m, 4 H), 7.28 - 7.33 (m, 4 H), 7.60 - 7.67 (m, 4 H), 8.14 - 8.23 (m, 4 H), 8.55 (d, *J*=4.13 Hz, 8 H). The electrospray mass spectrum in acetonitrile showed the peaks centered at *m/z*=919.35 corresponding to [M+H]<sup>+</sup> (calculated molecular mass=918.37). H<sub>2</sub>TANP displayed strong fluorescence at 655 nm, and 718 nm. The fluorescence lifetime of H<sub>2</sub>TANP was estimated to be 10.03 ns.

### Synthesis of ZnTANP

H<sub>2</sub>TANP, (27 mg, 0.03 mmol) was dissolved in 20 ml of chloroform in a 100 ml R.B. flask. A methanolic (10 ml) solution of Zn(OAc)<sub>2</sub>.2H<sub>2</sub>O (20 mg, 0.091 mmol) was added to this chloroform solution of the porphyrin. Then the mixture was refluxed for 2 h. The colour of the solution changes from purple to pink red during this process. The solvent mixture was removed by using a rotary evaporator. The crude product was dissolved in chloroform (60 ml) and was washed thoroughly with distilled water. Then the solution was dried by using anhydrous sodium sulphate and was purified by using silica gel column chromatography using CH<sub>2</sub>Cl<sub>2</sub> and hexane mixture as an eluent. The yield was 23mg (80%). Anal. Calcd (found) for C<sub>68</sub>H<sub>44</sub>N<sub>4</sub>Zn : C, 83.13 (83.28); H, 4.51 (4.64); N, 5.70 (5.85). UV-Vis (dichloromethane):  $\lambda_{\text{max}}/\text{nm}$  ( $\epsilon/\text{M}^{-1}\text{cm}^{-1}$ ): 428(371320), 550(22740), 588(3098). <sup>1</sup>H NMR (400 MHz, CHLOROFORM-*d*)  $\delta$  3.63-3.72 (m, 16 H), 6.82 - 7.00 (m, 4 H), 7.09 - 7.16 (m, 4 H), 7.27 - 7.28 (d, *J*=6.60 Hz, 4 H), 7.61 - 7.65 (m,

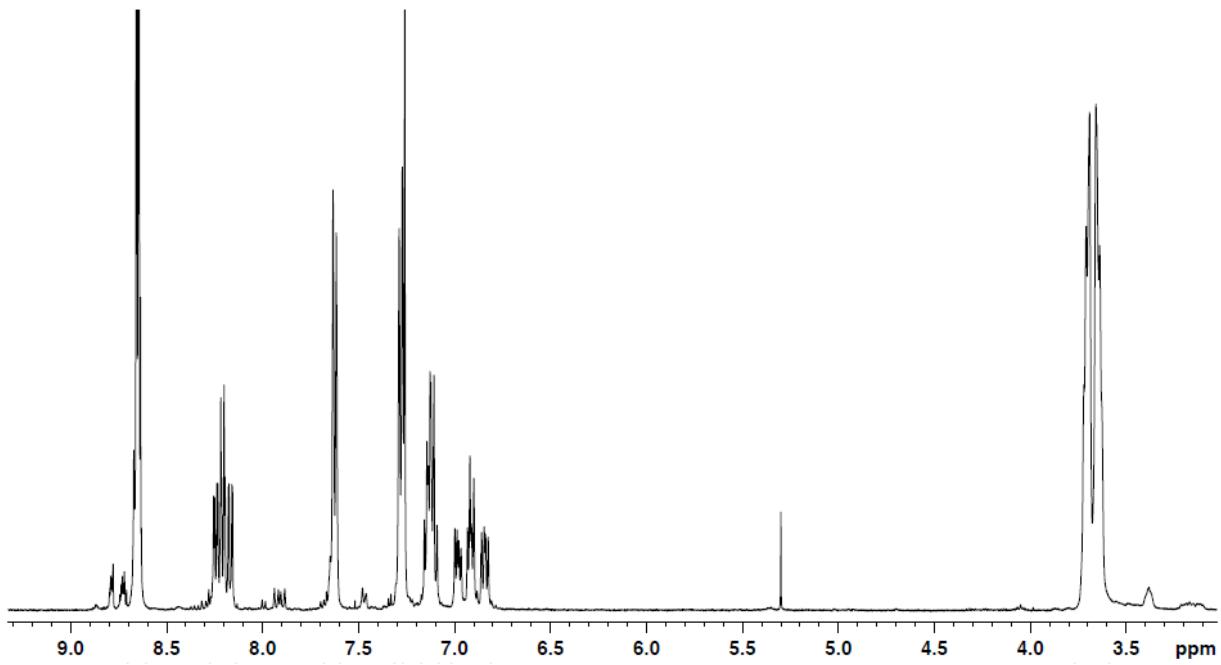
4 H), 8.15 - 8.26 (m, 4 H), 8.63 - 8.67 (m, 8 H). (Fig. S1)  $^{13}\text{C}$  NMR (101 MHz, CHLOROFORM-*d*)  $\delta$  151.16, 151.12, 151.10, 151.06, 146.33, 145.67, 138.66, 135.82, 135.34, 135.30, 134.60, 134.50, 134.47, 132.12, 128.17, 123.33, 123.29, 119.18, 118.45, 118.40, 118.05, 30.87, 30.57, 30.20, 29.86, 29.82, 29.52. The electrospray mass spectrum in acetonitrile (Fig. S2) showed the peaks centered at  $m/z$  = 980.86 corresponding to  $[\text{M}+\text{H}]^+$  (calculated molecular mass: 980.28). ZnTANP displayed strong fluorescence at 600 nm and 648 nm. The fluorescence lifetime of ZnTANP was estimated to be 1.02 ns.

**Figure Captions:**

**Fig. S1**  $^1\text{H}$  NMR spectrum of ZnTANP in  $\text{CDCl}_3$

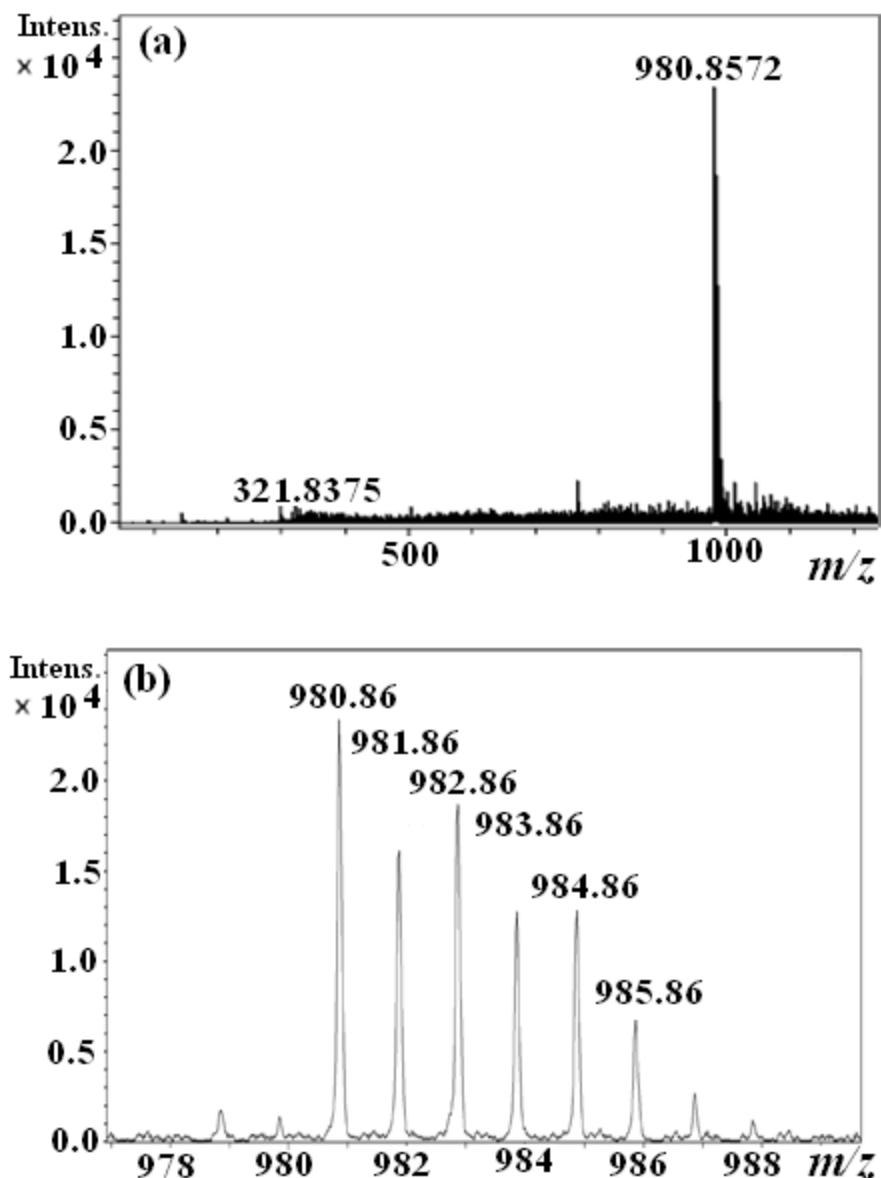
**Fig. S2** ESI- MS spectrum of ZnTANP in  $\text{CH}_3\text{CN}$  shows the (a) measured spectrum and (b) isotopic distribution pattern.

**Fig. S3** EDS spectrum of the  $\text{C}_{60}$ —ZnTANP circular disc grown on an *p*-Si substrate.

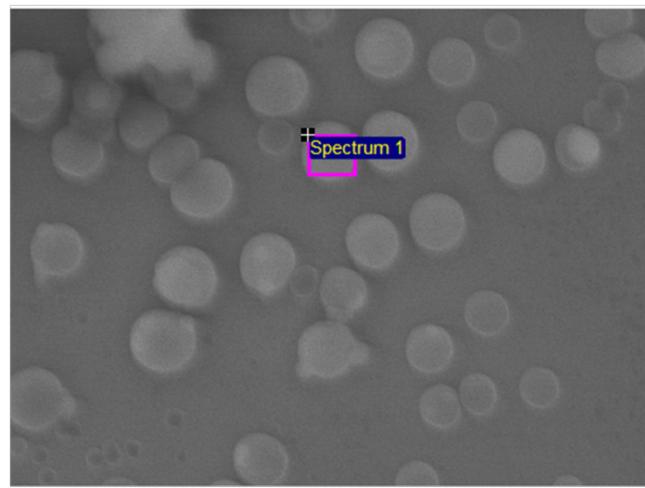


**Fig. S1**

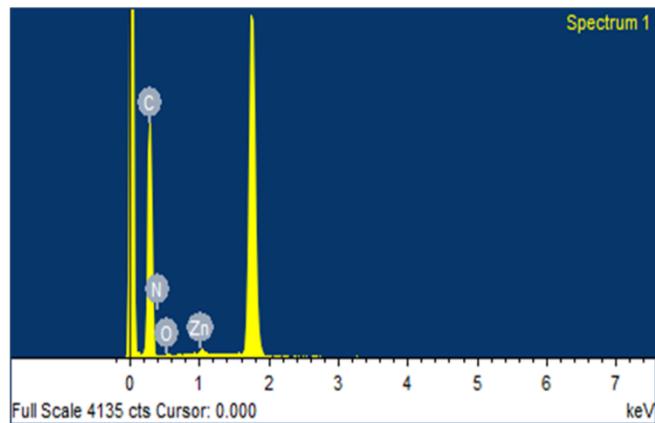
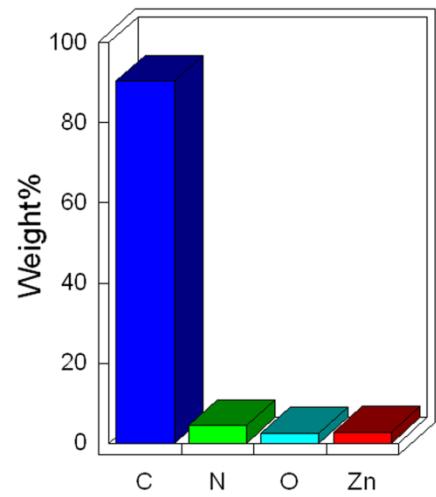
$^1\text{H}$  NMR spectrum of ZnTANP in  $\text{CDCl}_3$ .



**Fig. S2** ESI- MS spectrum of ZnTANP in  $\text{CH}_3\text{CN}$  shows the (a) measured spectrum and (b) isotopic distribution pattern.



Quantitative results



Element	Weight%
C	<b>90.32</b>
N	<b>4.43</b>
O	<b>2.46</b>
Zn	<b>2.79</b>

**Fig. S3** EDAX spectrum of the C<sub>60</sub>—ZnTANP circular disc grown on *p*-Si substrate.