Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplementary Information

Improved ternary memory performance of donor-acceptor structured molecules through cyano substitution

Qijian Zhang, Hao Zhuang, Jinghui He, Shugang Xia, Hua Li,* Najun Li, Qingfeng Xu and Jianmei Lu*

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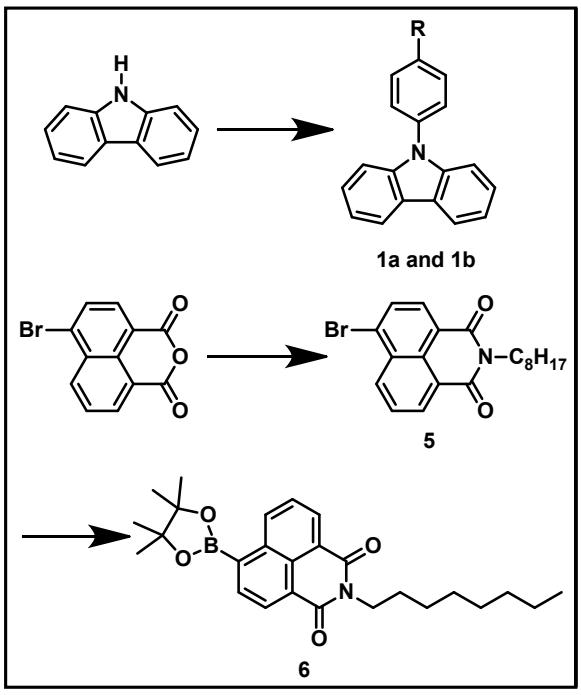

Scheme S1. Synthesis routes and molecular structures of the intermediates.

The two original compounds 9-phenyl-carbazole (1a), 4-(9H-carbazol-9-yl)benzonitrile (1b), 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-N-octyl-1,8-naphthalimide (6) were prepared according to previously reported procedures. [1-3]

Synthesis 2: Compound 2 was synthesized by the oxidative coupling reaction. To a 1000mL round flask were placed Iron (III) chloride (10.7 g, 66.0 mmol) and CH_2Cl_2 (400 mL) under N_2. To this mixture was very slowly added a solution of compound 1 (16.4 mmol) in CH_2Cl_2 (200 mL). The mixture was stirred at room temperature for 5 hour. After 10% sodium hydroxide solution was added in the mixture, the aqueous solution was thoroughly extracted with CH_2Cl_2. Then the crude product was dissolved in CH_2Cl_2 (10 mL) and reprecipitated slowly in methanol (400 mL). The product was collected by filtration and dried under vacuum at room temperature.

Compound 2a: yield 82%, white powder, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (s, 2H), 8.35 (d, 2H), 7.76 (d, 2H), 7.62 (d, 4H), 7.57 (d, 4H), 7.49 (m, J = 5.6 Hz, 6H), 7.29 (d, 2H), 7.25 (d, 2H).

Compound 2b: yield 80%, white powder, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (s, 2H), 8.24 (d, 2H), 7.94 (d, 4H), 7.80 (d, 6H), 7.56 (d, 2H), 7.50 (d, 4H), 7.38 (t, 2H).

Synthesis 3: compound 2 (6.0 mmol), NBS (2.3 g, 12.6 mmol) were added to 250 mL of $CHCl_3$ solution. The mixture was stirred at room temperature in dark for 12 h. The product was isolated by silicagel column chromatography using CH_2Cl_2: Hexane (v:v/1:5) as the eluent afford white solid.

Compound 3a: yield 91%, white powder, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (s, 2H), 8.36 (s, 2H), 7.78 (d, J = 8.5 Hz, 2H), 7.65 (t, J = 7.6 Hz, 4H), 7.58 (d, J = 7.3 Hz, 4H), 7.50 (d, J = 8.2 Hz, 6H), 7.31 (d, J = 8.7 Hz, 2H).

Compound 3b: yield 84%, white powder, ^{1}H NMR (400 MHz, DMSO) δ 8.82 (s, 2H), 8.65 (s, 2H), 8.18 (d, J = 8.4 Hz, 4H), 7.94 (d, J = 8.2 Hz, 6H), 7.63 – 7.59 (m, 4H), 7.49 (d, J = 8.7 Hz, 2H).

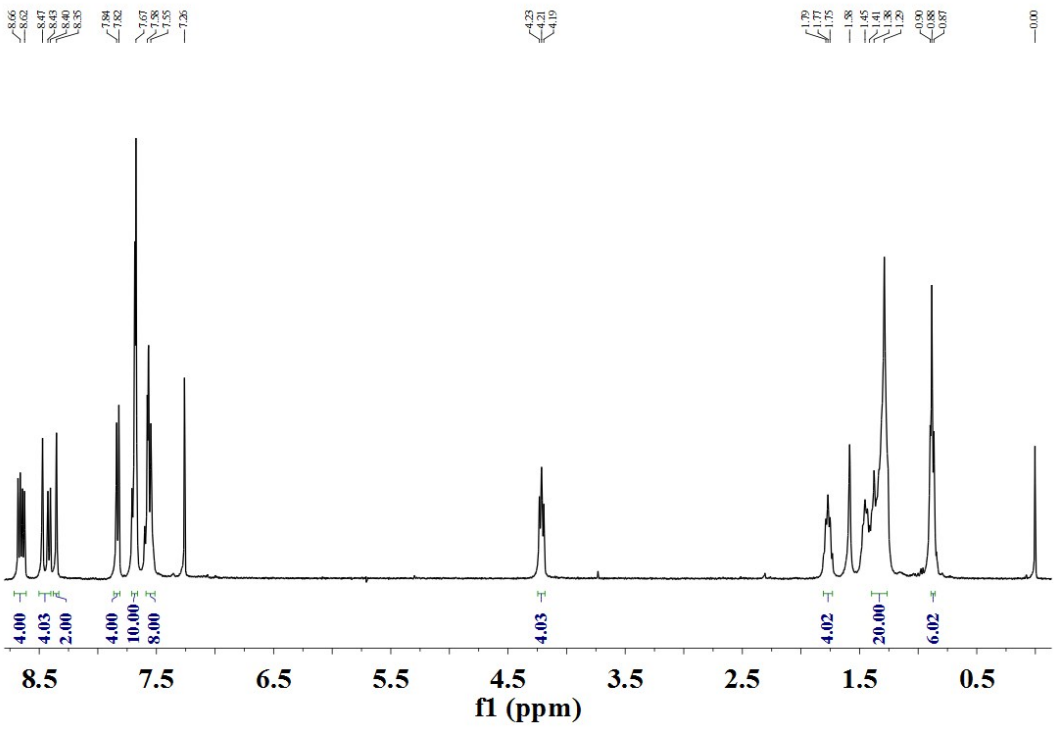

Figure S1. [1]H NMR spectra of DPHCANA.

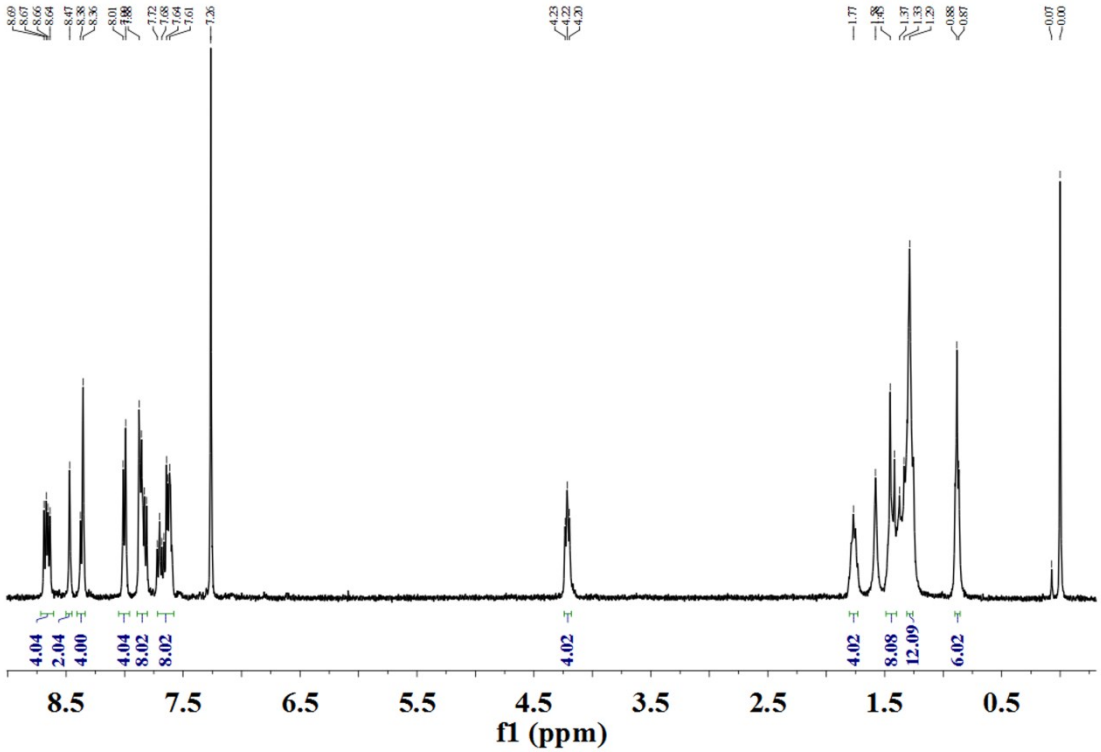

Figure S2.[1]H NMR spectra of DPCNCANA.

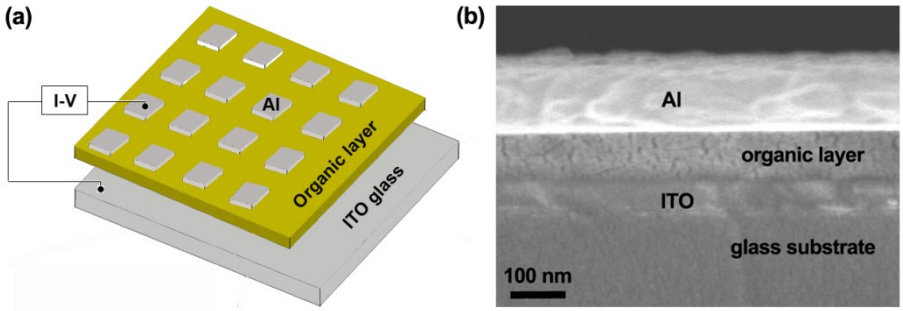

Figure S3. (a) The prototype of the sandwich-structured memory device; (b) SEM image of a cross section of the device.

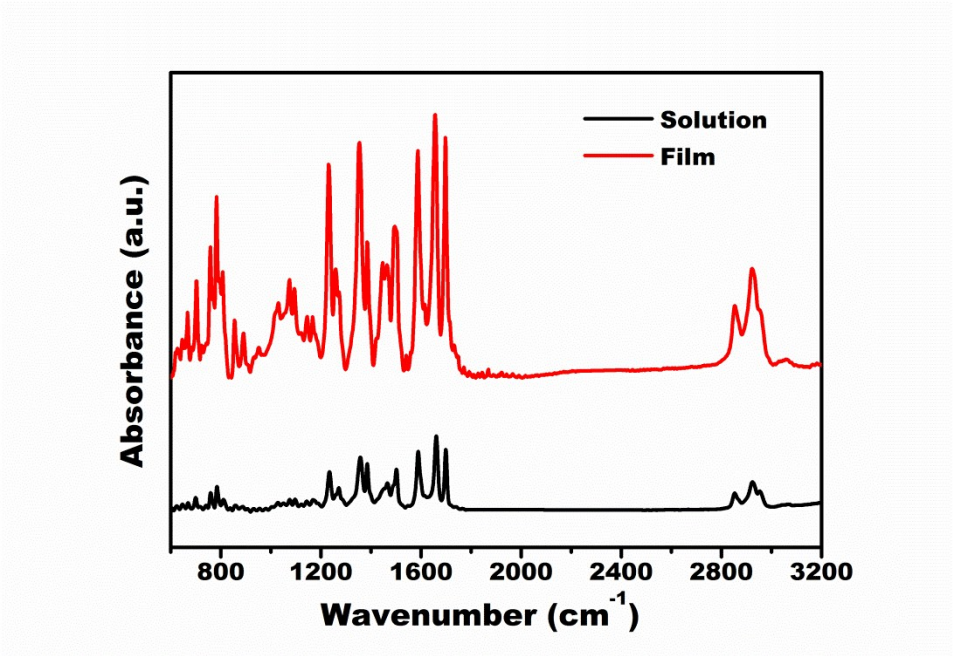

Figure S4. IR absorbance spectra of DPHCANA in solution and film states

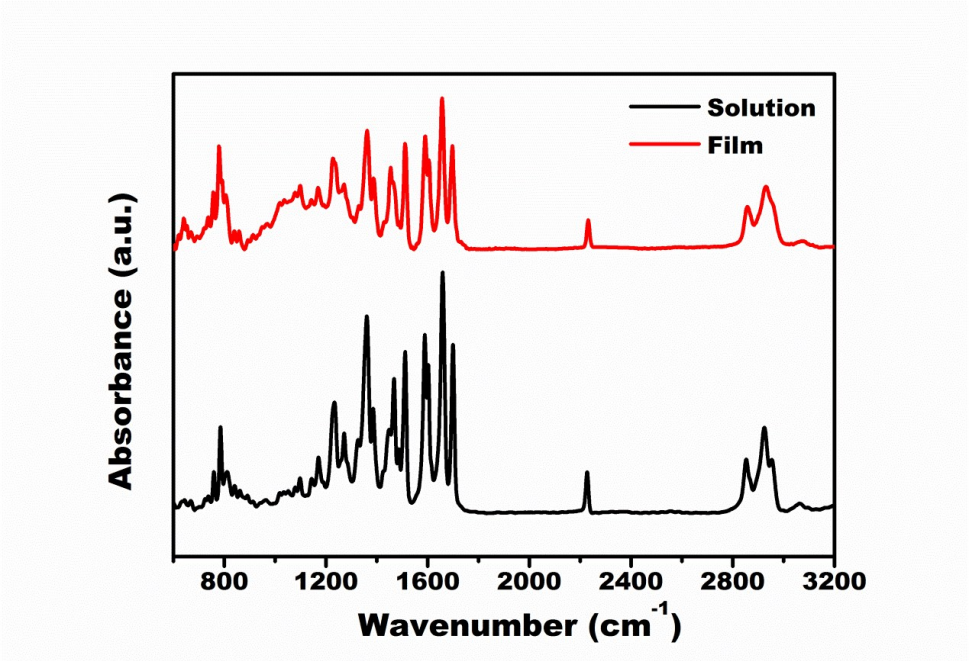

Figure S5. IR absorbance spectra of DPCNCANA in solution and film states

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