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

Supporting Information

Tuning Memory Performances from WORM to Flash or DRAM by Structural Tailoring with Different Donor Moieties

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1. ^{1}H NMR (DMSO-d_6) of HATT.

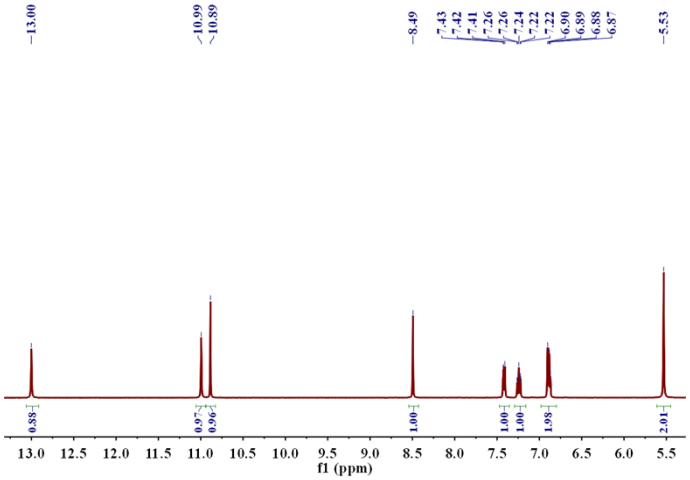

Figure S1. ^{1}H NMR (DMSO-d_6) of HATT.

2. The ^{13}C NMR spectrum of HATT in DMSO-*d6*.

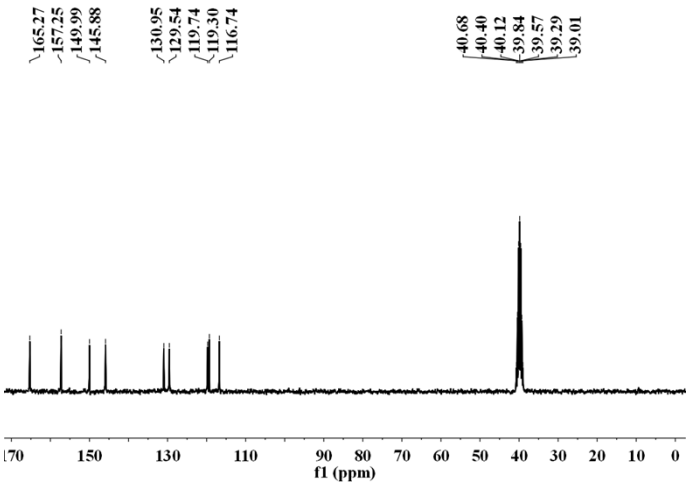

Figure S2. The ^{13}C NMR spectrum of HATT in DMSO-*d6*.

3. ^{1}H NMR (DMSO-d_6) of HDTT.

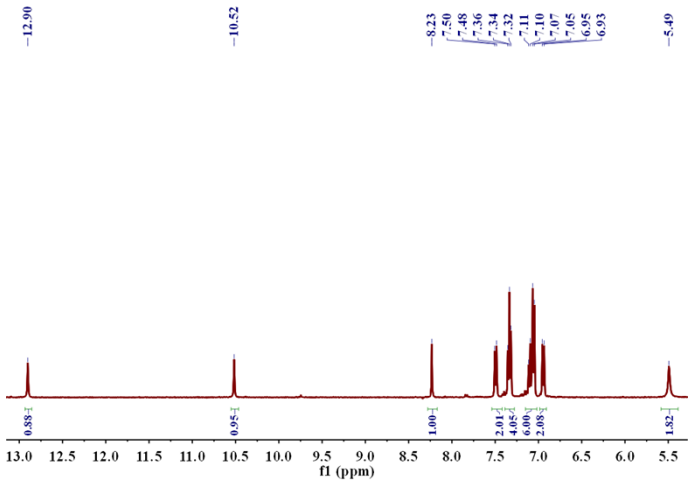

Figure S3. ^{1}H NMR (DMSO-d_6) of HDTT.

4. The ^{13}C NMR spectrum of HDTT in DMSO-*d6*.

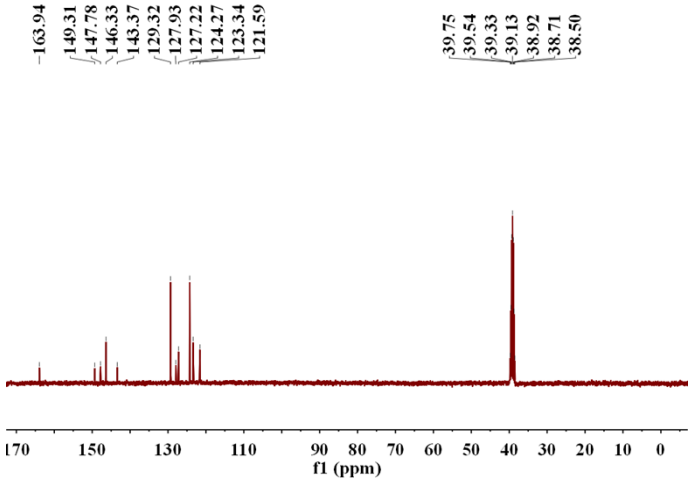

Figure S4. The ^{13}C NMR spectrum of HDTT in DMSO-*d6*.

5. The synthesis and characterization of HETT.

HETT and HRTT were synthesized by a similar procedure as HATT (Scheme 1). The crude product was purified by recrystallization from ethanol in 85 % yield. ^{1}H NMR (400 MHz, DMSO) δ 12.96 (s, 1H), 10.68 (s, 1H), 8.32 (s, 1H), 7.62 (d, J = 7.4 Hz, 2H), 7.51 – 7.26 (m, 3H), 5.52 ppm (s, 2H). ^{13}C NMR (75 MH_Z, [D6] DMSO): δ = 164.54, 149.73, 144.06, 134.80, 129.34, 128.85, 126.48 ppm; Elemental analysis calcd (%) for $C_9H_{10}N_6S$: C 46.14, H 4.30, N 35.87. Found: C 46.05, H 4.21, N 35.54.

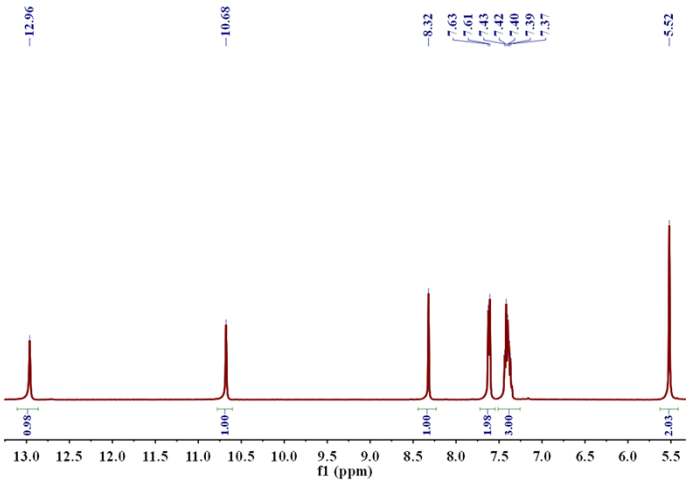

Figure S5. ^{1}H NMR (DMSO-d_6) of HETT.

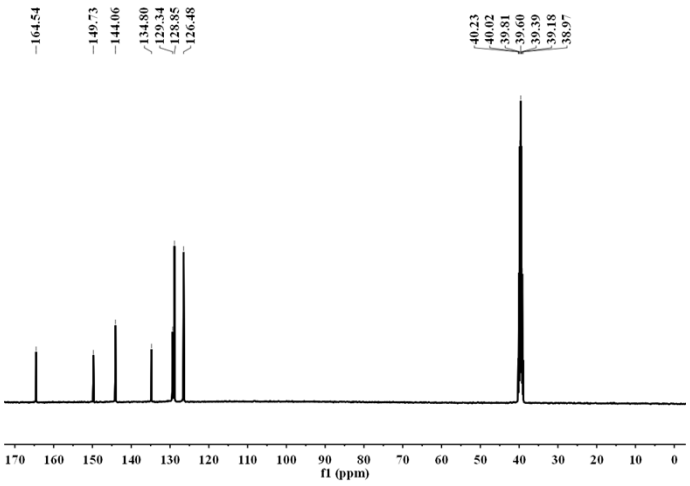

Figure S6. The ^{13}C NMR spectrum of HETT in DMSO-*d6*.

6. The synthesis and characterization of 4-(9*H*-carbazol-9-yl)benzaldehyde.

Carbazole (1.67g, 10 mmol), p-Fluorobenzaldehyde (1.24g, 10mmol), potassium carbonate (4.14g, 10 mmol), hexadecyl trimethyl ammonium bromide (0.0364 g, 0.1 mmol) and 50 mL DMF was added to a three-necked flask. After stirring for 3 days at 136 ^{o}C, the resulting mixture was poured into ice water and extracted with DCM. Removed the solvents by rotovap to give yellow powder. ^{1}H NMR (400 MHz, DMSO) δ 10.14 (s, 1H), 8.27 (d, J = 7.7 Hz, 2H), 8.21 (d, J = 8.2 Hz, 2H), 7.91 (d, J = 8.2 Hz, 2H), 7.53 (d, J = 8.2 Hz, 2H), 7.47 (t, J = 7.6 Hz, 2H), 7.34 ppm (t, J = 7.4 Hz, 2H).

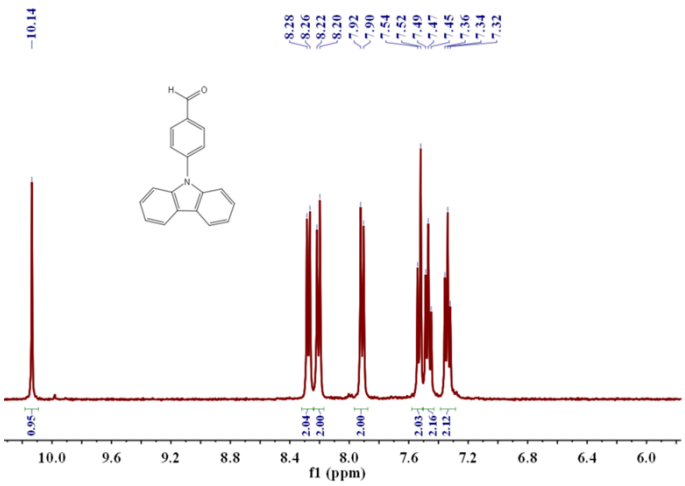

Figure S7. ^{1}H NMR (DMSO-d_6) of 4-(9*H*-carbazol-9-yl)benzaldehyde.

7. The synthesis and characterization of HRTT.

The crude product was purified by recrystallization from ethanol in 78% yield. ^{1}H NMR (400 MHz, DMSO) δ 13.02 (s, 1H), 10.84 (s, 1H), 8.47 (s, 1H), 8.26 (d, J = 7.7 Hz, 2H), 7.92 (d, J = 8.4 Hz, 2H), 7.69 (d, J = 8.4 Hz, 2H), 7.46 (d, J = 3.7 Hz, 4H), 7.32 (dd, J = 7.8, 4.0 Hz, 2H), 5.57 ppm (s, 2H). ^{13}C NMR (75 MH_Z, [D6] DMSO): δ = 164.62, 149.71, 143.10, 139.94, 137.45, 133.89, 128.08, 126.86, 126.44, 122.97, 120.68, 120.37, 109.83 ppm; Elemental analysis calcd (%) for $C_{21}H_{17}N_7S$: C 63.14, H 4.29, N 24.53. Found: C 63.09, H 4.19, N 24.59.

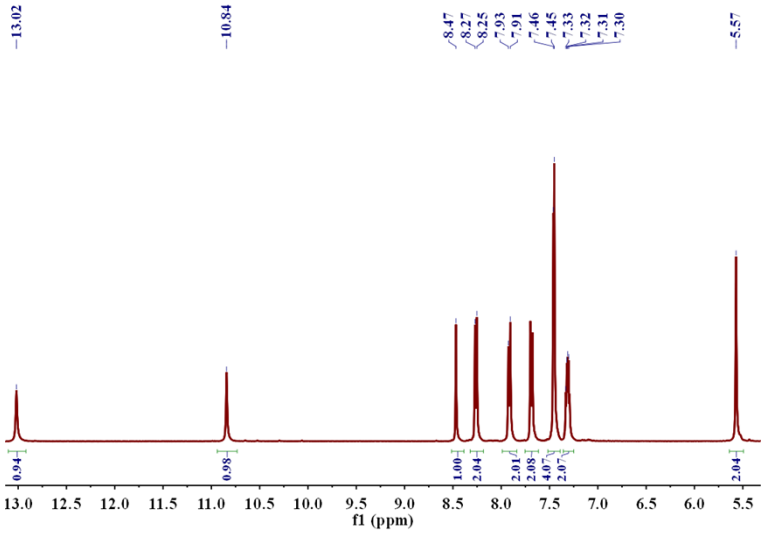

Figure S8. ^{1}H NMR (DMSO-d_6) of HRTT.

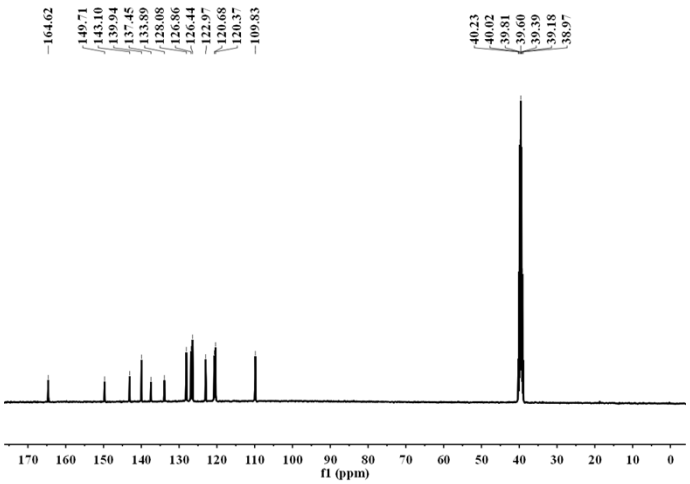

Figure S9. The ^{13}C NMR spectrum of HRTT in DMSO-*d6*.

8. TGA curves of four molecules.

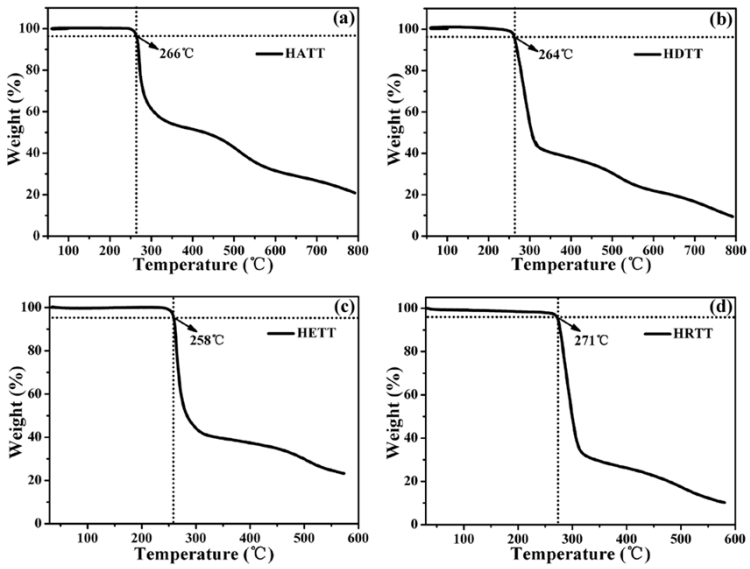

Figure S10. TGA curves of four small molecules: HATT (a), HDTT (b), HETT(c) and HRTT (d).

9. DSC curves of four molecules.

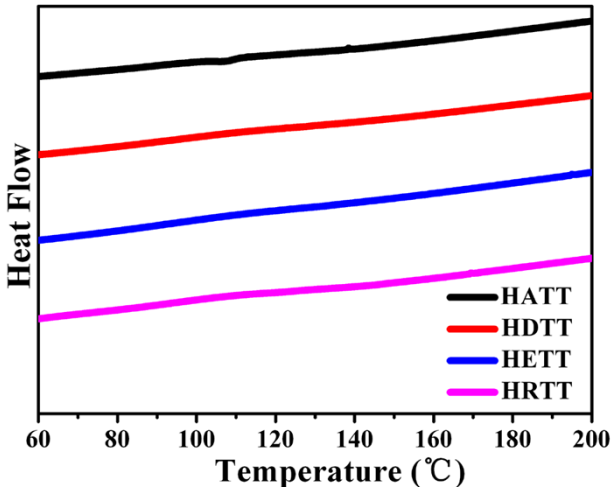

Figure S11. DSC curves of HATT, HDTT, HETT and HRTT.

10. Cyclic voltammograms of HATT, HDTT, HETT and HRTT films.

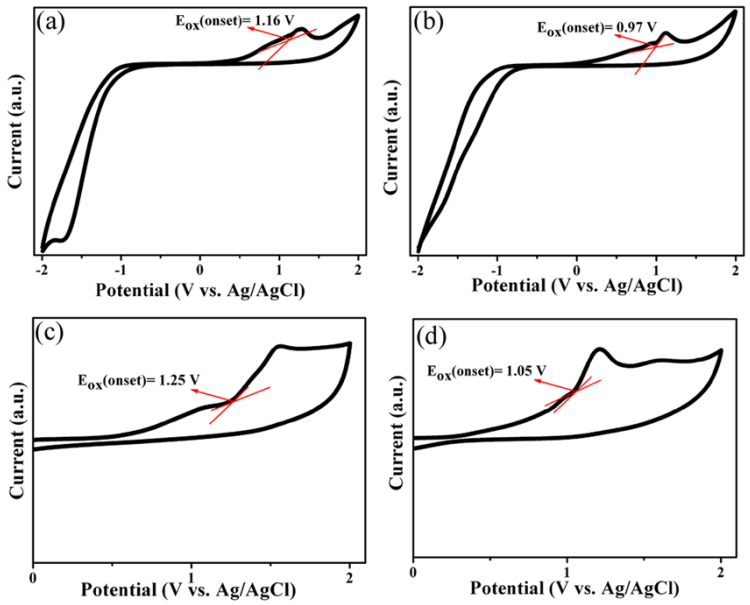

Figure S12. Cyclic voltammograms of (a) HATT, (b) HDTT, (c) HETT and HRTT on an ITO electrode in 0.1 M TBAP/CH_3CN solution with Ag/AgCl as reference electrode and Pt wire as counter electrode. A scan rate of 100mV/s was used.

11. XRD patterns of four films on quartz substrate.

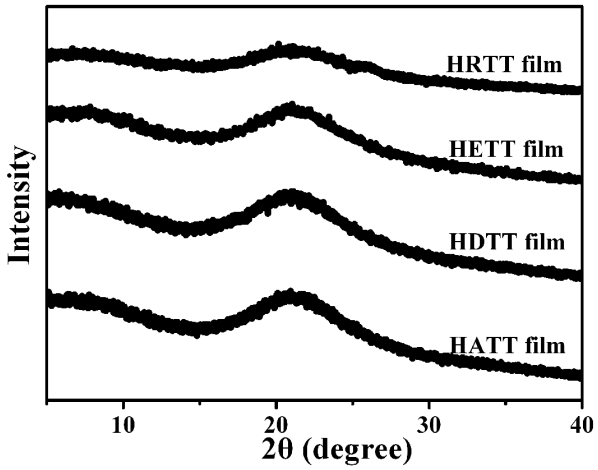

Figure S13. XRD patterns of HATT, HDTT, HETT and HRTT films on quartz substrate.

12. Cross-sectional SEM images of the devices.

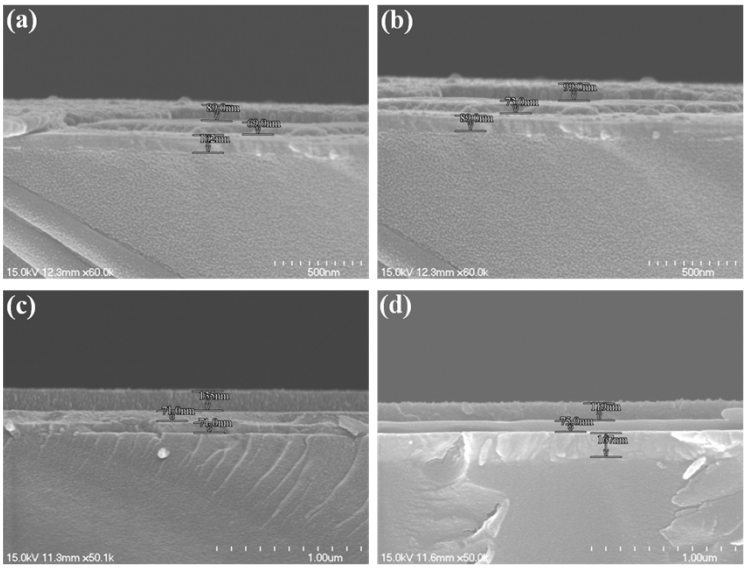

Figure S14. Cross-sectional SEM images of the ITO/HATT/Al (a), ITO/HDTT/Al (b), ITO/HETT/Al (c) and ITO/HRTT/Al (d) devices.

13. Values of orbital and system energies versus charges for the four molecules.

Table S1 Values of orbital and system energies versus charges for HATT.

Charge (M1)	HOMO (eV)	LUMO (eV)	Gap (eV)	Energy (eV)
-2	6.066	6.142	0.076	2.963
-1	1.291	1.811	0.52	-0.530
0	-4.627	-2.38	2.247	0.014
1	-8.769	-8.398	0.371	6.596
2	-12.739	-12.398	0.341	17. 180

Table S2 Values of orbital and system energies versus charges for HDTT.

Charge (M2)	HOMO (eV)	LUMO (eV)	Gap (eV)	Energy (eV)
-2	3.854	4.087	0.233	1.706
-1	0.758	1.128	0.37	-0.793
0	-4.515	-2.267	2.248	0
1	-7.609	-7.357	0.252	5.945
2	-10.869	-10.502	0.367	15.012

Table S3 Values of orbital and system energies versus charges for HETT.

Charge (M2)	HOMO (eV)	LUMO (eV)	Gap (eV)	Energy (eV)
-2	5.012	5.452	0.44	3.30
-1	1.27	1.803	0.533	0
0	-4.695	-2.445	2.25	0.6
1	-9.038	-8.628	0.41	7.3
2	-13.291	-12.711	0.58	18.1

Table S4 Values of orbital and system energies versus charges for HRTT.

Charge (M2)	HOMO (eV)	LUMO (eV)	Gap (eV)	Energy (eV)
-2	3.607	3.802	0.195	2.2
-1	-1.885	0.706	2.591	0
0	-4.762	-2.6	2.162	1.2
1	-7.78	-5.446	2.334	6.8
2	-11.001	-10.715	0.286	16.5