Electronic Supplementary Information

Controlled deposition of large-area and highly-ordered thin films: effect of dip-coating-induced morphological evolution on resistive memory performance

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Experimental Procedures

Materials

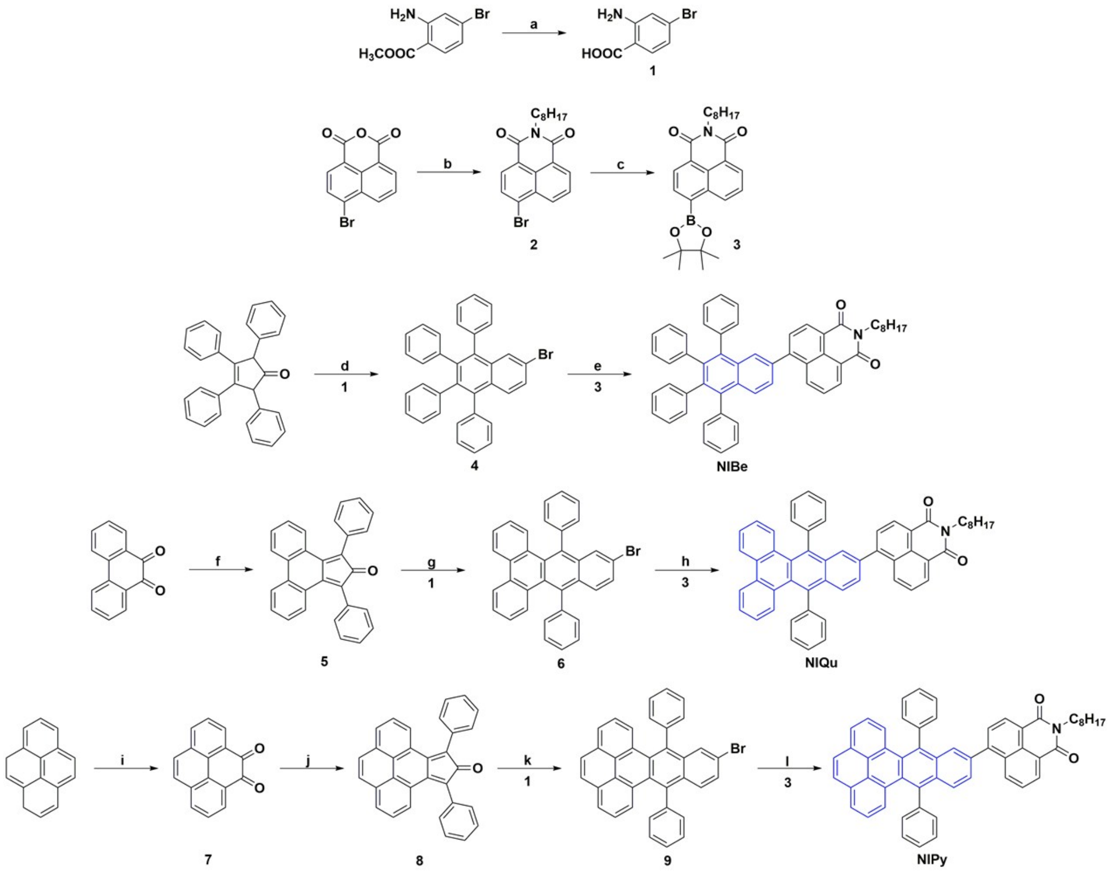
Methyl 2-amino-4-bromobenzoate, 4-bromo-1,8-naphthalic anhydride, *n*-octylamine, bis(pinacolato)diboron, 1,3-diphenyl-2-propanone, isoamyl nitrite, cyclopentadienone, phenanthrene-9,10-dione, pyrene, ruthenium(III) chloride hydrate ($RuCl_3 \cdot xH_2O$), sodium periodate ($NaIO_4$), and tetrakis(triphenylphosphine)palladium were purchased from Sigma-Aldrich company. 1,2-Dichloroethane (DCE) was distilled under argon atmosphere from calcium hydride and all other solvents and reagents were used as received without further purification.

Measurements and General Methods

Apparatus: All solution-state ^1H and ^{13}C NMR spectra in chloroform-*d* were acquired with a Bruker Advance 300 MHz NMR spectrometer unless otherwise noted. Data from elemental analysis were gotten by a Carlo-Erba EA-1110 instrument. Thermo gravimetric analysis (TGA) were conducted at a heating rate of 10 ºC min^{-1} with a TA instrument Dynamic TGA 2950 under a N_2 flow rate of 50 mL/min. UV–Vis absorption spectra were measured at room temperature with a Shimadzu UV-3600 spectrophotometer. Cyclic voltammograms (CVs) were collected using a three-electrode setup CorrTest CS Electrochemical Workstation analyzer in a solution of 0.1mol/L tetrabutylammonium hexafluorophosphate ($TBAPF_6$) in anhydrous dichloromethane at a sweep rate of 50 mV/s, with the assistances of a working electrode (Pt plate), a reference electrode Ag/AgCl, and a counter electrode (Pt wire), using Fc^+/Fc as an internal standard. The HOMO and LUMO were calculated using the following equation $E_{\mathrm{LUMO/HOMO}} = -e\,(4.80 - E_{\mathrm{Fc}} + E_{\mathrm{red/oxd}}^{\mathrm{onset}})$ V, where $E_{\mathrm{ox}}^{\mathrm{onset}}$ is the onset potential of the oxidation process and $E_{\mathrm{red}}^{\mathrm{onset}}$ is the onset potential of the reduction process.[S1,S2] Dip-coating was conducted by a SYDC-100H DIP COATER instrument. Atomic force microscopy (AFM) measurements were performed to study the morphology of dip-coated films with a MFP-3DTM (Digital Instruments/Asylum Research) AFM instrument, in which topographical and phase images were obtained concurrently. Density functional theory (DFT) was performed using the generalized gradient approximation (GGA) in DMol3 code at unrestricted BLYP/DNP set.

Single-crystal X-ray diffraction: The yellow plate-like crystals of **NIPy** were obtained by slow evaporation of mixed solvents (chloroform/isopropanol = 2:1). During the single crystal growth process, 3.0 mg **NIPy** was firstly dissolved into 2.0 mL chloroform in a small bottle, then 1.0 mL isopropanol was carefully added onto the top of chloroform (v/v = 2/1). After slowly evaporating for about 3−4 days under ambient conditions, the yellow plate-like crystals started to appear at the bottom of bottle. The suitable single crystal was selected for single-crystal X-ray data collection with a Bruker SMART APEX-II CCD area detector on a D8 goniometer. The data were collected using graphite-monochromated and Mo-Kα radiation (λ = 0.71073 Å) with the ω scan method[S3] at 103 K. The data were processed with the SAINT program of the APEX3 software for reduction and cell refinement. Multi-scan absorption corrections were applied by using the SADABS program for area detector. All structures were solved by the direct method and refined by the full-matrix least-squares method on F^2 (SHELXL-2016/6).[S4] All non-H atoms were refined anisotropically. Crystallographic data and structural refinements are summarized in Table S1. CCDC 1870372 contains the supplementary crystallographic data for this paper. The crystal packing mode of **NIPy** shows that two adjacent molecules form a dimer and the chloroform solvent molecule is incorporated. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Synthesis



Scheme S1. Synthetic routine of **NIBe**, **NIQu** and **NIPy**. (a) NaOH/methanol, 86%; (b) *n*-octylamine/ethanol, 78%; (c) bis(pinacolato)diboron/KOAc/toluene, 60%; (d) isoamyl nitrite/1,2-dichloroethane, 47%; (e) K_2CO_3/H_2O/toluene/ethanol/$Pd(PPh_3)_4$, 52%; (f) 1,3-diphenyl-2-propanone/NaOH/methanol, 77%; (g) isoamyl nitrite/1,2-dichloroethane, 48%; (h) K_2CO_3/H_2O/toluene/ethanol/$Pd(PPh_3)_4$, 61%; (i) $RuCl_3 \cdot xH_2O/NaIO_4/CH_2Cl_2/CH_3CN/H_2O$, 60%; (j) 1,3-diphenyl-2-propanone /NaOH/ethanol, 53%; (k) isoamyl nitrite/1,2-dichloroethane, 39%; (l) K_2CO_3/H_2O/toluene/ethanol/$Pd(PPh_3)_4$, 70%.

Synthesis of 2-amino-4-bromobenzoic acid (1)[S5]

A round-bottom flask containing methyl 2-amino-4-bromobenzoate (2.30 g, 10.0 mmol) was mixed with 2 N NaOH (35.6 mL) and methanol (35.6 mL). The mixture was heated at reflux overnight. After cooling to room temperature for 10 min, water (100 mL) was added to the flask and the solution was titrated to pH = 6 with 1 N HCl. The solution was further cooled in an ice bath for 30 min. The precipitate was filtered, washed with cold water (3 × 50 mL) and dried in vacuo overnight to give compound **1** (1.86 g, 8.61 mmol, 86%) as pale yellow solid.

^{1}H NMR (300 MHz, DMSO) δ (ppm): 7.59 (d, J = 8.5 Hz, 1H), 6.97 (d, J = 1.9 Hz, 1H), 6.64 (dd, J = 8.5, 2.0 Hz, 1H).

Synthesis of 6-bromo-2-octyl-1H-benzo[de]isoquinoline-1,3(2H)-dione (2) 4-Bromo-1,8-naphthalic anhydride (2.50 g, 9.03 mmol), *n*-octylamine (2.32 g, 18.0 mmol) and anhydrous ethanol (200 mL) were added into a single-neck round-bottom flask connected with a condenser. The mixture was maintained at 78 °C to reflux overnight until the color of the solution became dark, and then cooled to precipitate. The resulting suspension was filtered and washed with cold ethanol twice to obtain light yellow crude product. The crude material was purified by column chromatography on silica gel to yield white solid **2** (2.73 g, 7.03 mmol, 78%).

^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.62 (d, J = 7.3 Hz, 1H), 8.52 (d, J = 8.5 Hz, 1H), 8.38 (d, J = 7.8 Hz, 1H), 8.00 (d, J = 7.8 Hz, 1H), 7.82 (t, J = 7.9 Hz, 1H), 4.14 (t, J = 7.0 Hz, 2H), 1.71 (m, 2H), 1.43 – 1.26 (m, 10H), 0.86 (t, J = 6.5 Hz, 3H).

Synthesis of 2-octyl-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (3)

Under protection of argon, compound **2** (1.55 g, 4.00 mmol), bis(pinacolato)diboron (B_2pin_2) (1.52 g, 6.00 mmol) and anhydrous potassium acetate (1.18 g, 12.0 mmol) were dissolved into anhydrous toluene (50 mL). The mixture was degassed for 20 min, then dichloro[1,1'-bis(diphenylphosphino)-ferrocene]palladium(II) (290 mg, 0.40 mmol) was added quickly and the mixture was degassed for another 10 min. After the reaction mixture was heated at 70 °C for 16 h, it was extracted with dichloromethane and washed with distilled water. The organic extract was dried over sodium sulfate, and solvent was removal under reduced pressure yielded brown viscous oil. Purification by column chromatography on silica gel using CH_2Cl_2/hexane ether as eluent yielded white solid **3** (1.04 g, 2.39 mmol, 60%).

^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 9.12 (d, J = 7.5 Hz, 1H), 8.60 (m, 2H), 8.32 (d, J = 7.9 Hz, 1H), 7.79 (d, J = 7.9 Hz, 1H), 7.82 (t, J = 7.9 Hz, 1H), 4.18 (t, J = 7.1 Hz, 2H), 1.74 – 1.16 (m, 24H), 0.88 (t, J = 6.6 Hz, 3H).

Synthesis of 6-bromo-1,2,3,4-tetraphenylnaphthalene (4)[S6]

Compound **1** (432 mg, 2.00 mmol) in 1,2-dichloroethane (35 mL) was added dropwise to a boiling solution of cyclopentadienone (769 mg, 2.00 mmol) and isoamyl nitrite (2.0 mL, 14.3 mmol) in 1,2-dichloroethane (35 mL) under an Ar atmosphere. The reaction was heated at reflux overnight. Then the solution was cooled down, and the solvent was evaporated under vacuum. After passing through a silica column using CH_2Cl_2/hexane as eluent, a pale-yellow product (476 mg, 0.93 mmol, 47%) was obtained.

^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 7.78 (d, J = 1.8 Hz, 1H), 7.54 – 7.41 (m, 2H), 7.29 – 7.26 (m, 1H), 7.25 – 7.14 (m, 9H), 6.90 – 6.78 (m, 10H).

Synthesis of 1,3-diphenyl-2H-cyclopenta[l]phenanthren-2-one (5)[S7]

Phenanthrene-9,10-dione (1.50 g, 7.20 mmol) was added to 1,3-diphenyl-2-propanone (1.60 g, 7.60 mmol) in dry methanol (90 ml) in a two-necked round bottom flask fitted with a water-cooled condenser and a dropping funnel containing a solution of methanolic potassium hydroxide (0.40 g KOH in 1.60 ml) in dry methanol. The reaction mixture was stirred while heating. The methanolic potassium hydroxide solution was added dropwise once the methanol began to reflux. The reaction was further refluxed for 15 min. Upon chilling, the obtained black powder was filtered and washed with cold methanol, dried in vacuo overnight to yield the compound **5** (2.12 g, 5.54 mmol, 77%).

^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 7.81 – 7.69 (m, 2H), 7.55 – 7.48 (m, 2H), 7.44 – 7.27 (m, 10H), 7.24 (s, 2H), 6.95 – 6.89 (m, 2H).

Synthesis of 11-bromo-9,14-diphenylbenzo[f]tetraphene (6)

Reaction Condition was similar with that for compound **4**, except compound **5** (762 mg, 2.00 mmol) was used. Purification of the crude material on silica gel by CH_2Cl_2/hexane as eluent yielded the compound **6** (487 mg, 0.96 mmol, 48%).

^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.26 (d, J = 7.1 Hz, 2H), 8.07 (d, J = 1.9 Hz, 1H), 7.79 (d, J = 9.2 Hz, 1H), 7.59 – 7.45 (m, 13H), 7.40 – 7.30 (m, 2H), 6.98 (t, J = 7.4 Hz, 2H).

Synthesis of pyrene-4,5-dione (7)[S8]

To a solution of pyrene (2.04 g, 10 mmol) in CH_2Cl_2 (40.0 mL) and CH_3CN (40.0 mL), $NaIO_4$ (10.0 g, 46.8 mmol), H_2O (50.0 mL), and $RuCl_3 \cdot xH_2O$ (0.20 g, 0.96 mmol) were added. The dark brown suspension was stirred at room temperature overnight. The reaction mixture was poured into 500 mL of H_2O and the organic phase was separated. The aqueous phase was extracted with CH_2Cl_2 (3 × 50 mL). The combined organic phase was evaporated under reduced pressure to afford a dark orange solid. After passing through a silica column using CH_2Cl_2/hexane as eluent, compound **7** (1.40 g, 6.03 mmol, 60%) was obtained as bright orange crystals.

^1H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.47 (d, J = 7.9 Hz, 2H), 8.16 (d, J = 7.5 Hz, 2H), 7.82 (s, 2H), 7.84 – 7.72 (m, 2H).

Synthesis of 9,11-diphenyl-10H-cyclopenta[e]pyren-10-one (8)[S9]

Compound **7** (2.19 g, 9.45 mmol) and 1,3-diphenyl-2-propanone (2.20 g, 10.5 mmol) were mixed in ethanol (65 mL). A solution of KOH (95 mg) in ethanol (20 mL) was added dropwise until all of the compound **7** dissolved. The solution was then heated in a hot water bath, and the remainder of the base was added. Red-brown crystals began to form on the sides of the flask, and after a brief reflux, the mixture was cooled to 0 °C. The crystalline product was filtered and dried in vacuo overnight to afford compound **8** (2.04 g, 5.02 mmol, 53%).

^1H NMR (300 MHz, $CDCl_3$) δ (ppm): 7.86 (d, J = 7.5 Hz, 2H), 7.72 (d, J = 7.6 Hz, 2H), 7.65 (s, 2H), 7.45 (s, 10H), 7.31 – 7.20 (m, 2H).

Synthesis of 11-bromo-9,14-diphenyldibenzo[de,qr]tetracene (9)

Reaction Condition was similar with that for compound **4**, except compound **8** (813 mg, 2.00 mmol) was used. Purification of the crude material on silica gel by CH_2Cl_2/hexane as eluent yielded the compound **9** (418 mg, 0.78 mmol, 39%).

^1H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.06 (d, J = 1.9 Hz, 1H), 7.91 – 7.83 (m, 4H), 7.82 – 7.45 (m, 3H), 7.59 – 7.47 (m, 11H), 7.33 (t, J = 7.9 Hz, 2H).

Synthesis of 2-octyl-6-(5,6,7,8-tetraphenylnaphthalen-2-yl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (NIBe)

Compound **4** (307 mg, 0.60 mmol), compound **3** (392 mg, 0.90 mmol) and anhydrous potassium carbonate (166 mg, 1.2 mmol) were charged with a three-neck round-bottom flask, cycled with argon protection and dissolved in toluene (20 mL), distilled water (20 mL) and anhydrous ethanol (8 mL). The mixture was degassed for 20 min before tetrakis(triphenylphosphine)palladium (70.0 mg, 0.06 mmol) was added quickly. The reaction mixture was subsequently degassed again for another 10 min, and then heated at 70 °C under argon for 24 h. The reaction mixture was allowed to cool down to room temperature, after which it was extracted with dichloromethane and washed with distilled water. The organic extract was dried over sodium sulfate, and then collected by rotary vacuum. The crude material was purified by column chromatography on silica gel with a mixed mobile phase of CH_2Cl_2/hexane to yield product **NIBe** as pale yellow solid (230 mg, 0.31 mmol, 52%).

^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.60 (d, J = 7.5 Hz, 2H), 8.29 – 8.17 (m, 1H), 7.88 – 7.60 (m, 2H), 7.54 (d, J = 8.7 Hz, 1H), 7.33 – 7.26 (m, 5H), 7.25 – 7.06 (m, 5H), 6.86 (d, J =6.9 Hz, 10H), 4.23 – 4.14 (m, 2H), 1.79 – 1.67 (m, 2H), 1.40 – 1.26 (m, 10H), 0.90 – 0.85 (m, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 164.30, 164.07, 146.86, 140.24, 140.00, 139.92, 139.24, 139.03, 138.82, 138.52, 136.24, 133.81, 132.57, 131.96, 131.67, 131.25, 131.21, 131.14, 130.78, 130.14, 128.69, 128.33, 128.03, 127.70, 127.64, 127.52, 127.49, 126.69, 125.54, 122.97, 121.79, 40.51, 31.83, 29.36, 29.24, 28.15, 27.16, 22.64, 14.09.

Elemental analysis (%) calcd for $C_{54}H_{45}NO_2$: C, 87.65; H, 6.13; N, 1.89; found: C, 85.73; H, 6.41; N, 1.69.

Synthesis of 6-(9,14-diphenylbenzo[f]tetraphen-11-yl)-2-octyl-1H-benzo[de]isoquinoline-1,3(2H)-dione (NIQu)

Reaction Condition was similar with that for **NIBe**, except compound **6** (306 mg, 0.60 mmol) was used. Purification of the crude material on silica gel by CH_2Cl_2/hexane as eluent yielded the product **NIQu** as light yellow solid (270 mg, 0.37 mmol, 61%).

^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.62 (d, J = 8.6 Hz, 2H), 8.34 (dd, J = 22.1, 8.1 Hz, 3H), 8.16 – 8.00 (m, 2H), 7.80 – 7.32 (m, 17H), 7.08 – 6.95 (m, 2H), 4.26 – 4.15 (m, 2H), 1.81 – 1.68 (m, 2H), 1.44 – 1.26 (m, 10H), 0.89 – 0.85 (m, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) *δ* (ppm): 164.32, 164.11, 146.96, 141.45, 141.30, 135.95, 135.72, 135.39, 132.68, 132.58, 132.46, 132.08, 131.60, 131.28, 131.18, 131.12, 131.06, 130.82, 130.56, 130.14, 129.96, 129.17, 128.15, 127.86, 127.31, 127.15, 126.78, 125.94, 123.40, 123.05, 121.83, 40.54, 31.84, 29.38, 29.25, 28.18, 27.19, 22.65, 14.09.

Elemental analysis (%) calcd for $C_{54}H_{43}NO_2$: C, 87.89; H, 5.87; N, 1.90; found: C, 86.08; H, 6.25; N, 1.60.

Synthesis of 6-(9,14-diphenyldibenzo[de,qr]tetracen-11-yl)-2-octyl-1H-benzo[de]isoquinoline-1,3(2H)-dione (NIPy)

Reaction Condition was similar with that for **NIBe**, except compound **9** (320 mg, 0.60 mmol) was used. Purification of the crude material on silica gel by CH_2Cl_2/hexane as eluent yielded the product **NIPy** as yellow solid (320 mg, 0.42 mmol, 70%).

^{1}H NMR (300 MHz, $CDCl_3$) *δ* (ppm): 8.64 (d, *J* = 7.5 Hz, 2H), 8.39 (d, *J* = 8.4 Hz, 1H), 8.15 – 8.01 (m, 2H), 7.96 – 7.81 (m, 6H), 7.73 (dd, *J*=14.8, 7.6 Hz, 2H), 7.67 – 7.30 (m, 13H), 4.25 – 4.16 (m, 2H), 1.82 – 1.67 (m, 2H), 1.41 – 1.26 (m, 10H), 0.90 – 0.85 (m, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) *δ* (ppm): 164.32, 164.11, 146.94, 141.96, 141.80, 136.83, 136.50, 136.04, 132.67, 132.37, 132.24, 131.83, 131.51, 131.18, 130.80, 130.14, 130.06, 129.28, 129.24, 128.85, 128.79, 128.30, 128.14, 127.80, 127.42, 126.91, 126.78, 126.14, 125.96, 124.81, 123.06, 121.85, 40.54, 31.84, 29.38, 29.25, 28.18, 27.19, 22.65, 14.09.

Elemental analysis (%) calcd for $C_{56}H_{43}NO_2$: C, 88.27; H, 5.69; N, 1.84; found: C, 85.08; H, 6.14; N, 1.48.

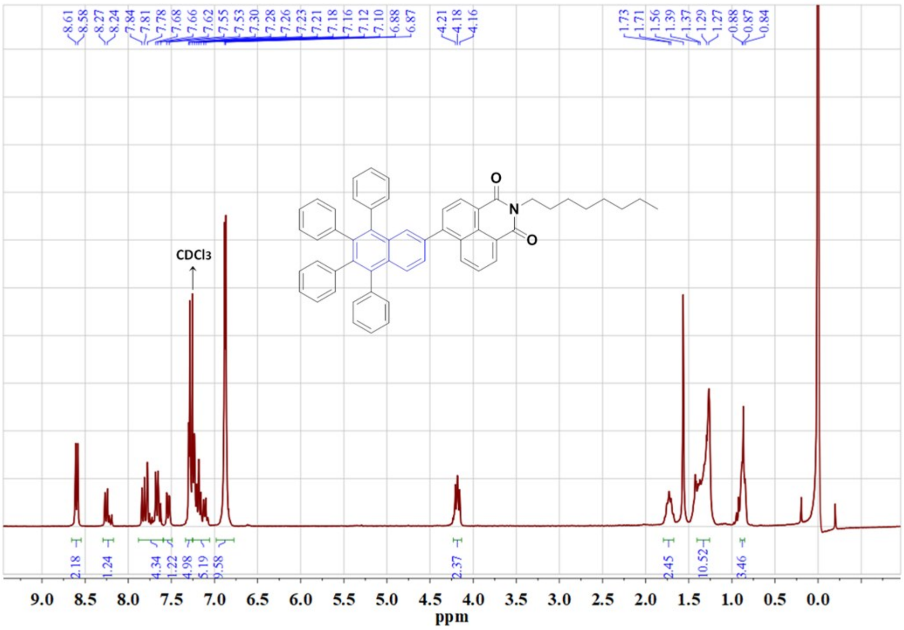


Figure S1. ^{1}H NMR spectrum of **NIBe** in $CDCl_3$.

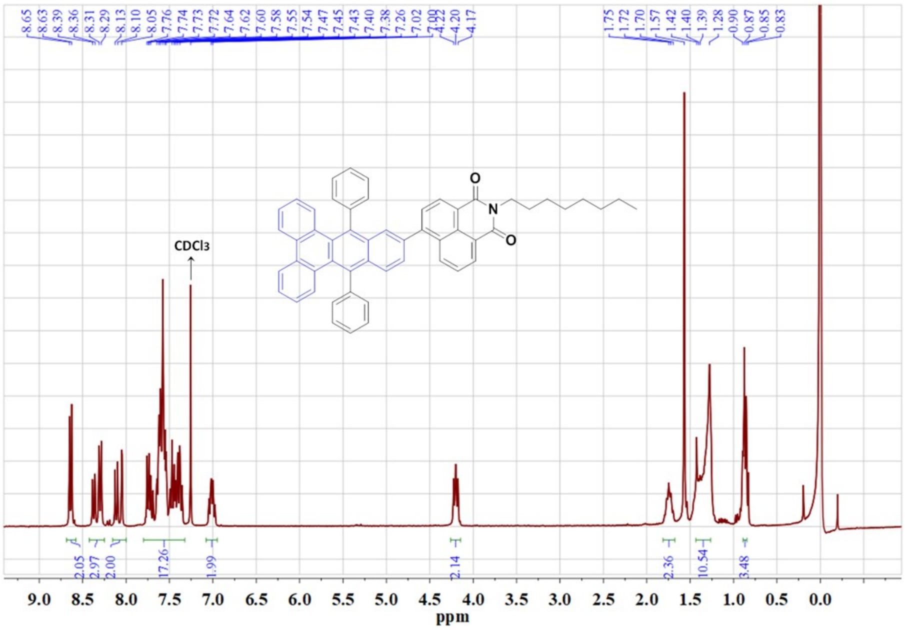


Figure S2. ^{1}H NMR spectrum of **NIQu** in $CDCl_3$.

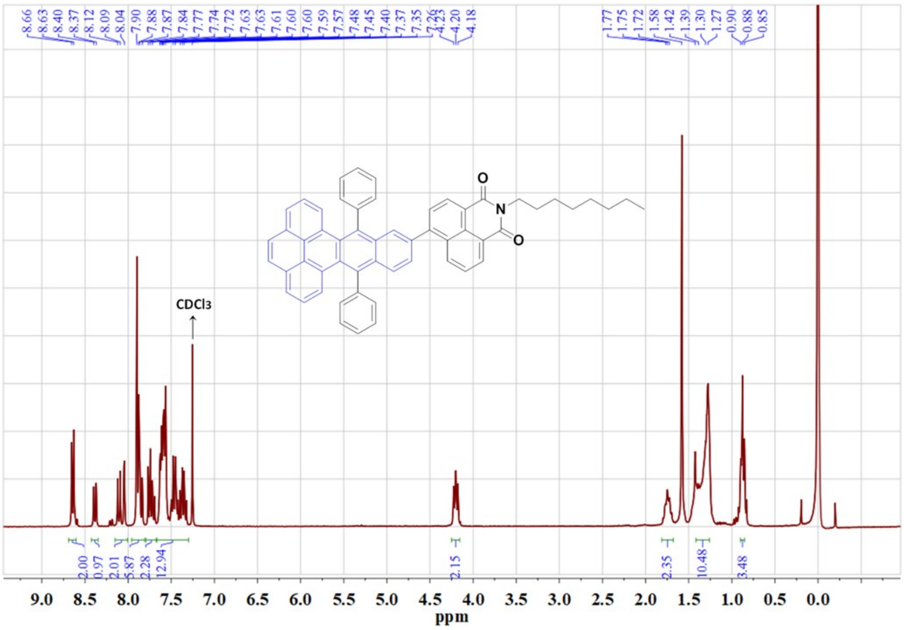


Figure S3. ^{1}H NMR spectrum of **NIPy** in $CDCl_3$.

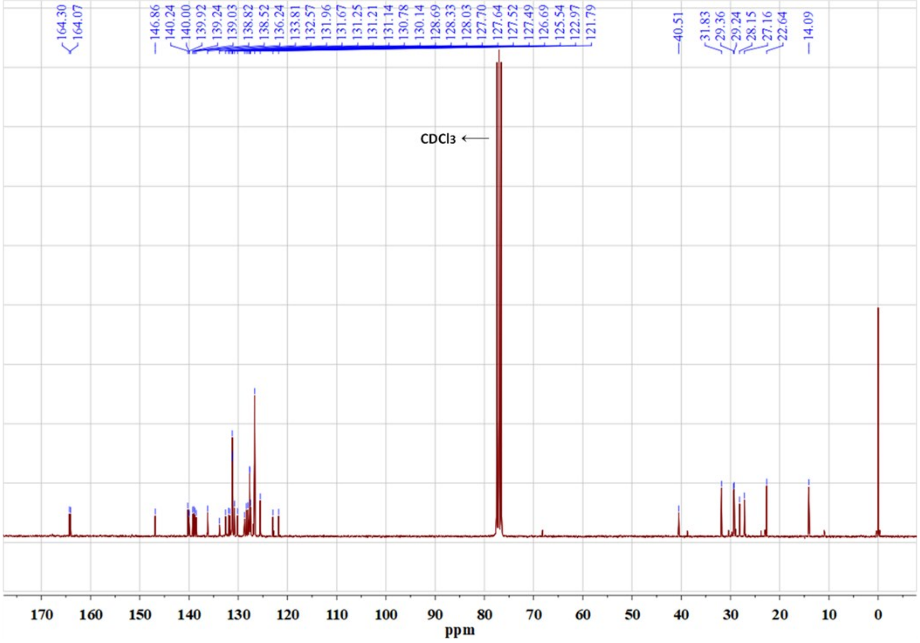


Figure S4. ^{13}C NMR spectrum of **NIBe** in $CDCl_3$.

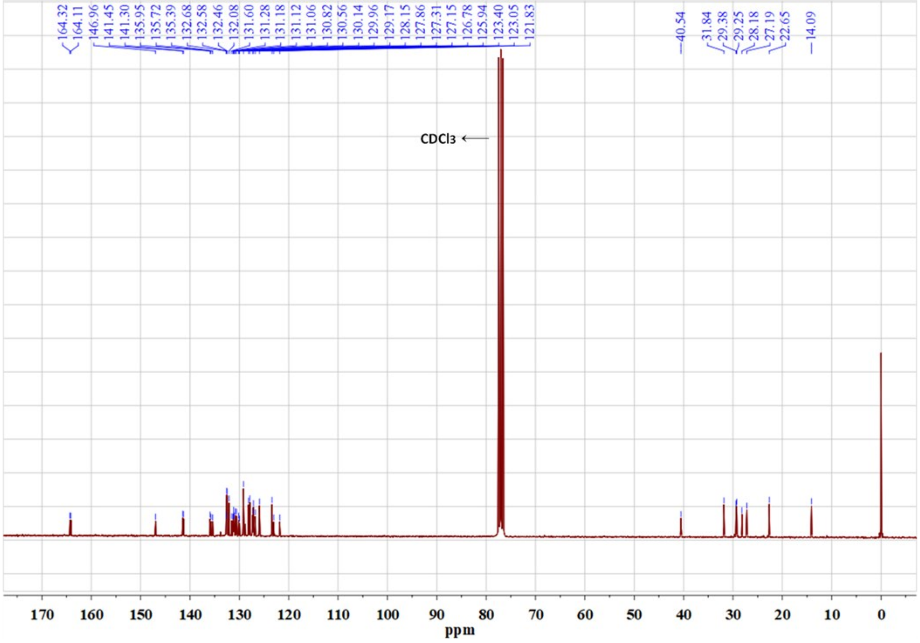


Figure S5. ^{13}C NMR spectrum of **NIQu** in $CDCl_3$.

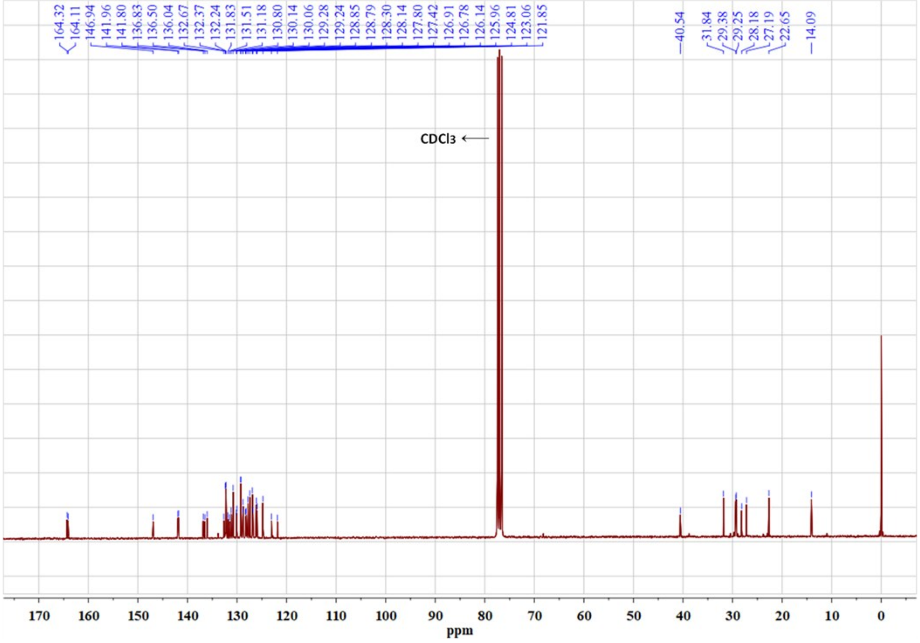


Figure S6. ^{13}C NMR spectrum of **NIPy** in $CDCl_3$.

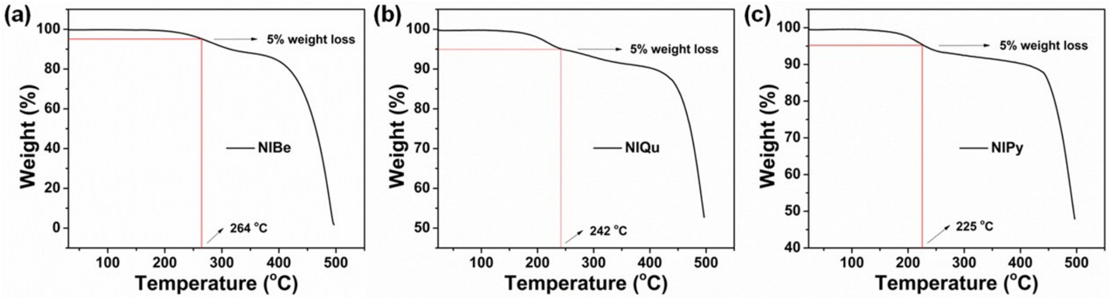


Figure S7. TGA curves of (a) **NIBe**, (b) **NIQu** and (c) **NIPy** at a heating rate of 10 ºC min^{-1} under a nitrogen atmosphere.

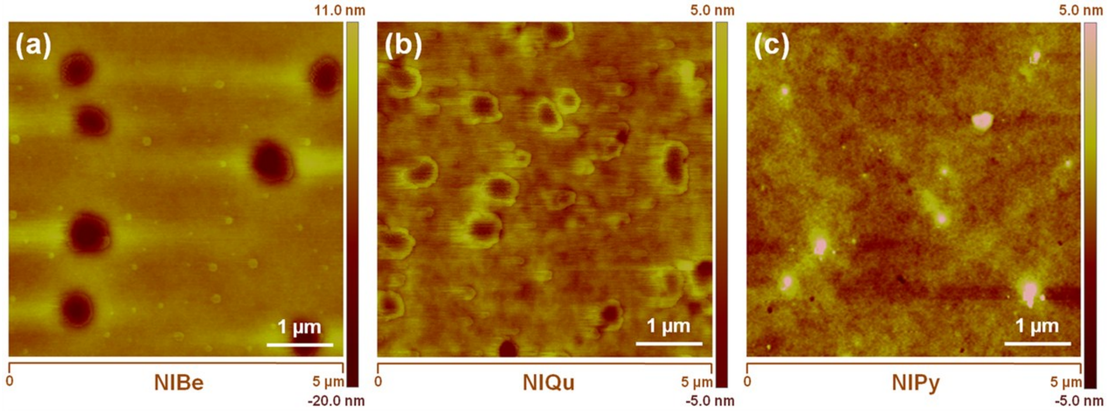


Figure S8. AFM images of (a) **NIBe**, (b) **NIQu** and (c) **NIPy** spin-coated thin films on ITO substrates.

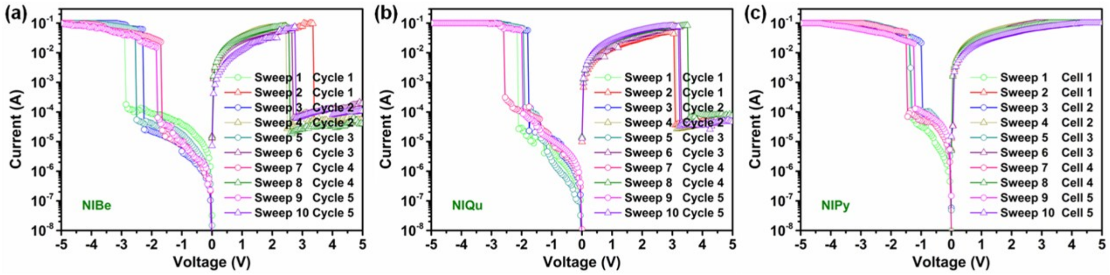


Figure S9. Repeatable current–voltage characteristics of (a) **NIBe**, (b) **NIQu** and (c) **NIPy** based memory devices.

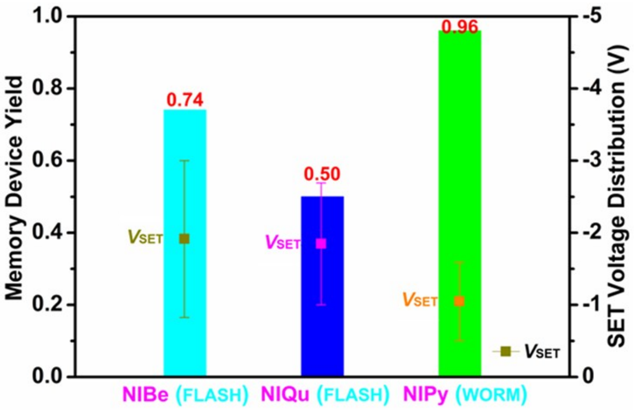


Figure S10. The statistical reproducibility (shown by column-chart plot) and the SET voltage (V_{SET}) distributions of **NIBe**, **NIQu** and **NIPy** based OMDs (shown by error bar).

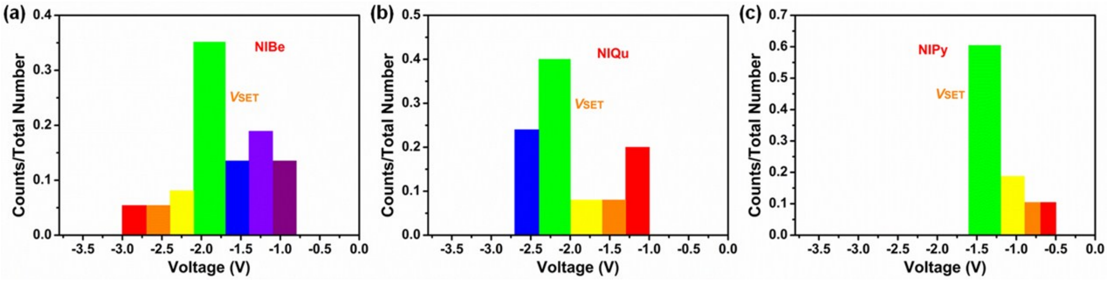


Figure S11. The detailed V_{SET} distributions of (a) **NIBe**, (b) **NIQu** and (c) **NIPy** based OMDs shown by column-chart plot; from **NIBe** to **NIPy**, the distribution tends to be more centralized in narrower range.

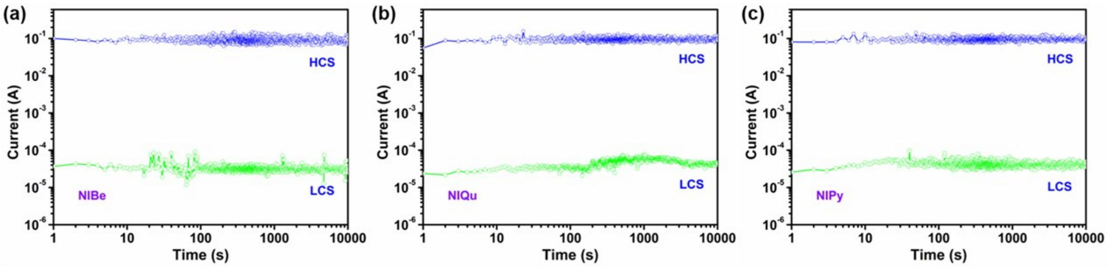


Figure S12. Retention time test of (a) **NIBe**, (b) **NIQu** and (c) **NIPy** based dip-coated OMDs in both LCS and HCS under a constant “read” voltage of –1.0 V; the current states were well-separated with narrow fluctuations within one order of magnitude.

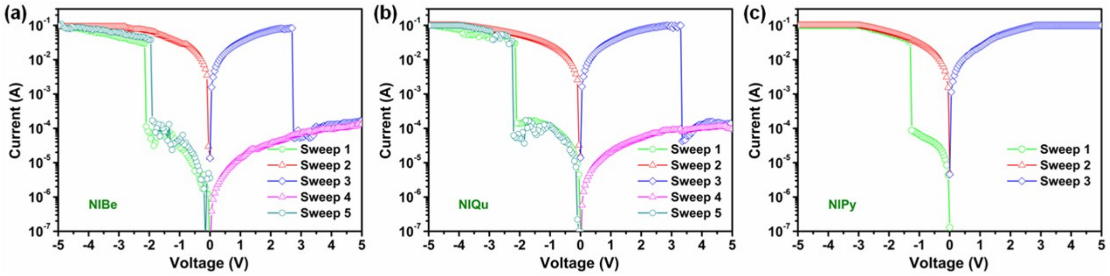


Figure S13. Current–voltage characteristics of (a) **NIBe**, (b) **NIQu** and (c) **NIPy** based memory devices with ITO/small-molecule/Au structure.

Table S1. Crystallographic data and structure refinement parameters of **NIPy**

	NIPy
T (K)	103(2)
Formula	$C_{113}H_{87}Cl_3N_2O_4$
Formula weight	1643.19
Crystal system	triclinic
Space group	*P -1*
Z	2
a (Å)	9.7201(4)
b (Å)	20.7651(7)
c (Å)	22.6267(8)
α (deg)	87.0396(13)°
β (deg)	83.6537(13)°
γ (deg)	80.6042(13)°
V (Å^3)	4475.4(3)
ρ calcd (g/cm3)	1.219
λ (Mo Kα) (Å)	0.71073
Collected reflns	61873
Unique reflns	15824
Parameters	1145
R (int)	0.1313
R1 [$I > 2\sigma(I)$]	0.0886
wR2 [$I > 2\sigma(I)$]	0.2978
GOF	1.040

Table S2. Detailed sweep profile and parameters of the device testing

Test Name	res2t#1@1	
Mode	Sweeping	
Speed	Normal	
Sweep Delay	0	
Hold Time	0	
Site Coordinate	0,0	
KTEI Version	V9.0 SP1	
Interlock	High Voltage Disabled	
Device Terminal	B	A
Instrument	SMU1	SMU2
Name	BV	AV
Forcing Function	Voltage Bias	Voltage Sweep
Master/Slave	N/A	Master
Start/Level	0	0
Stop	N/A	-5 V or 5 V
Step	N/A	0.05 V
Number of Points	4096	101
Compliance	0.1 A	0.1 A
Measure I	Measured	Measured
Measure V	No	Programmed
Range I	Auto	Auto
Range V	Best Fixed	Best Fixed
Range C	N/A	N/A
AC Voltage	N/A	N/A
Over Voltage Setting	OFF	OFF
Formulas	RES = AVG(AV/AI)	

Table S3. Optical and electrochemical properties of **NIBe**, **NIQu** and **NIPy**

	λ_{max} (nm)		λ_{onset} (nm)	$E_{g(opt)}$[c]	$E_{ox(CV)}$[d]	$E_{red(CV)}$[e]	HOMO[f]	LUMO[g]	$E_{g(CV)}$[h]
compound	solution[a]	film[b]	film[b]	[eV]	[eV]	[eV]	[eV]	[eV]	[eV]
NIBe	352	468	553	2.24	1.08	–0.87	–5.46	–3.51	1.95
NIQu	358	439	549	2.26	1.34	–0.94	–5.72	–3.44	2.28
NIPy	332	433	547	2.27	1.33	–0.90	–5.71	–3.48	2.23

[a] In ODCB solution at 10^{-4} M; [b] Dip-coated thin film; [c] Estimated from the absorption onset of the thin film: $E_{g(opt)} = 1240/\lambda_{onset}$; [d,e] Vs Ag/AgCl; [f] Determined by the onset of the oxidation peak of CVs; [g] Determined by the onset of the reduction peak of CVs; [h] Estimated from CVs.

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