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Supporting Information

Different interaction between metal electrode and organic layer and their different

electrical bistability performances

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1. ¹H NMR and ¹³C NMR of 2PyNI



Figure S1. ¹H NMR spectrum of **2PyNI** in DMSO-*d6*.



Figure S2. ¹³C NMR spectrum of 2PyNI in CF₃COOD.

2. Thermo-gravimetric Analysis (TGA) for bulk powder of 2PyNI.

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Figure S3. TGA curve of 2PyNI.

The thermal stabilities of **2PyNI** were evaluated by TGA under a nitrogen atmosphere. As shown in the TGA curves, the thermal decomposition temperatures (the 5% weight-lost temperature) of **2PyNI** 5 was up to 297 °C, respectively. The good-thermal stability of **2PyNI** would endure heat deterioration in the memory devices.

3. Scanning Electron Microscope (SEM) images of the devices



Figure S4. The cross section images of devices: (a) ITO/2PyNI/Au; (b) ITO/2PyNI/Al.

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4. High resolution mass spectrometry (HRMS) of 2PyNI

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Figure S5. HRMS spectrum of 2PyNI.

5. Crystallographic data of 2PyNI

5 Table S1. Crystallographic data for 2PyNI

Compound	2PyNI	
Formula	$C_{24}H_{20}N_6O_4$	
F_w	456.46	
T(K)	223(2)	
Crystal system	orthorhombic	
Space group	P 21 21 21	
a (Å)	4.6051(10)	
b (Å)	13.887(3)	
c (Å)	33.216(7)	
a (deg)	90	
β (deg)	90	
γ (deg)	90	
V(Å ³)	2124.1(8)	

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Ζ	4
D _{calc}	1.427
$\mu(mm^{-1})$	0.101
F (000)	952
θ_{max} (deg)	27.44
Reflections Collected	11621
Independent reflections	4749
Observed reflections	3398
Parameters refined	320
$R(I \ge 2\sigma(I))$	0.0681
wR ₂ (all data)	0.1490
GOF on F ²	1.102

6. The extended retention time characterization of device 2



5 Figure S6. The effect of retention time of the memory device under a constant stress of -1.0 V

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7. The Temperature dependence characterization of device 1 and 2 for ON sate

Figure S7. Temperature dependence of the current for the ON states of devices 1 and 2.

The temperature dependence (between 250 and 320 K) of the current for ON state of device 1 and 2 5 were measured. The current was subsequently measured at 1 V while the temperature was swept at a speed of 1.0 K/min. It was found that the current for ON state of device 1 and 2 did not show the feature of conductors and was weakly affected by the temperature.