# Electronic Supplementary Information

## Well-Defined Star-Shaped Donor-Acceptor Conjugated Molecules for Organic Resistive Memory Devices

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# Experimental

## Materials and Characterizations

Two studied star-shaped D-A molecules, TPA-T-NI and TPA-3T-NI, were prepared according to the previous report.[S1] Anhydrous chloroform for device fabrication were purchased from Aldrich (Missouri, USA) and used without further purification. The thickness of polymer film was measured with a Microfigure Measuring Instrument (Surfcorder ET3000, Kosaka Laboratory Ltd.). The surface morphology of the studied materials was explored using a Nanoscope 3D Controller atomic force microscopy (AFM, Digital Instruments (Santa Barbara, CA)) operated in the tapping mode at room temperature, and commercial silicon cantilevers with typical spring constants of 21-78 N $m^{-1}$ were used.

## Fabrication and Measurement of Data Storage Devices

The resistive data storage device was fabricated from the studied molecules with a cross-point sandwiched configuration, Al/active material/Al. The substrate (i.e. Si wafer) was firstly cleaned with nitrogen stream and washed with toluene, acetone, and isopropanol, in that order. 30-nm thick Al bottom electrode patterns were deposited by a thermal evaporator at a pressure of $10^{-6}$ torr with a depositing rate of 1 Å $s^{-1}$. Then, 5 mg $ml^{-1}$ of the studied materials in chloroform was filtered through 0.22 μm pore size of PTFE membrane syringe filter, spin-coated onto the bottom Al electrode at 1000 rpm for 60 s and baked at 100 $^{o}$C on a hot plate in $N_2$-filled glove

box to remove the solvent residue. Finally, the 45-nm Al top electrodes was thermally deposited and patterned by a shadow mask with cross-point device joint area. The electrical properties of the memory device was carried out by a Keithley 4200-SCS semiconductor parameter analyzer in a nitrogen-filled glove box at room temperature.

**Computational Methodology**

Theoretical molecular simulation of ground state structures for TPA-T-NI and TPA-3T-NI is performed with the Gaussian 03 program package and investigated using density functional theory (DFT) method. The B3LYP functional is used in conjunction with 6-31G(d) basis set.[S2] Note that the alkyl chains on TPA-3T-NI were truncated to methyl groups to save the computing.

## References

S1. J. Zhang, G. Li, C. Kang, H. Lu, X. Zhao, C. Li, W. Li and Z. Bo, *Dyes Pigm.*, 2015, **115**, 181.

S2. *Gaussian 03*, *revision B.04*, Gaussian, Inc., Wallingford, CT, 2004.

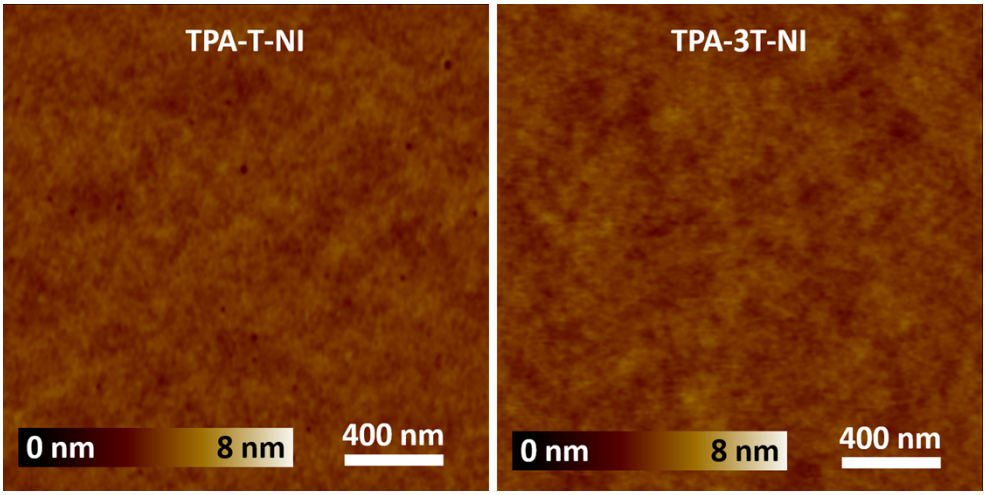


**Fig. S1.** Tapping mode AFM topographies of spin-coated TPA-T-NI and TPA-3T-NI thin films on Si wafer from chloroform solutions. The surface roughness is 0.23 and 0.25 nm of TPA-T-NI and TPA-3T-NI thin film, respectively.

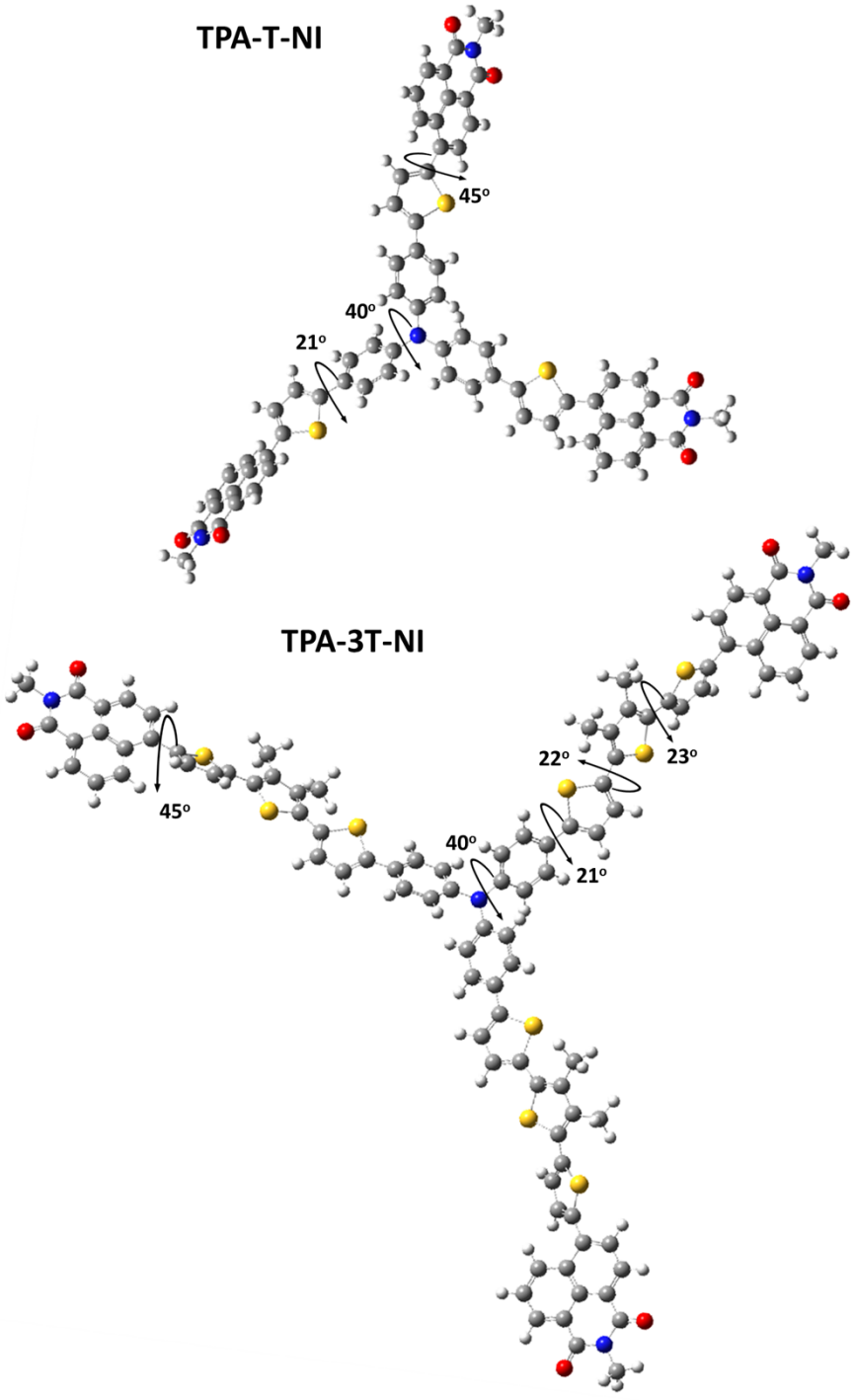


**Fig. S2.** Optimized molecular geometry of TPA-T-NI and TPA-3T-NI. The alkyl side chains were replaced with the methyl groups to simplify the calculation.