

**Supporting information for**  
**First-principles study of phthalocyanine-based multifunctional spintronic**  
**molecular device**

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Table S1. Magnetic moments of central TMPc molecules for the devices at 0 V. A positive value means the TMPc molecule is spin-up polarized while a negative value means the TMPc molecule is spin-down polarized.

Molecular Device	M1	C1	M2	C2	M3
Magnetic Moment ( $\mu_B$ )	3.079	3.789	-3.093	-3.745	3.086

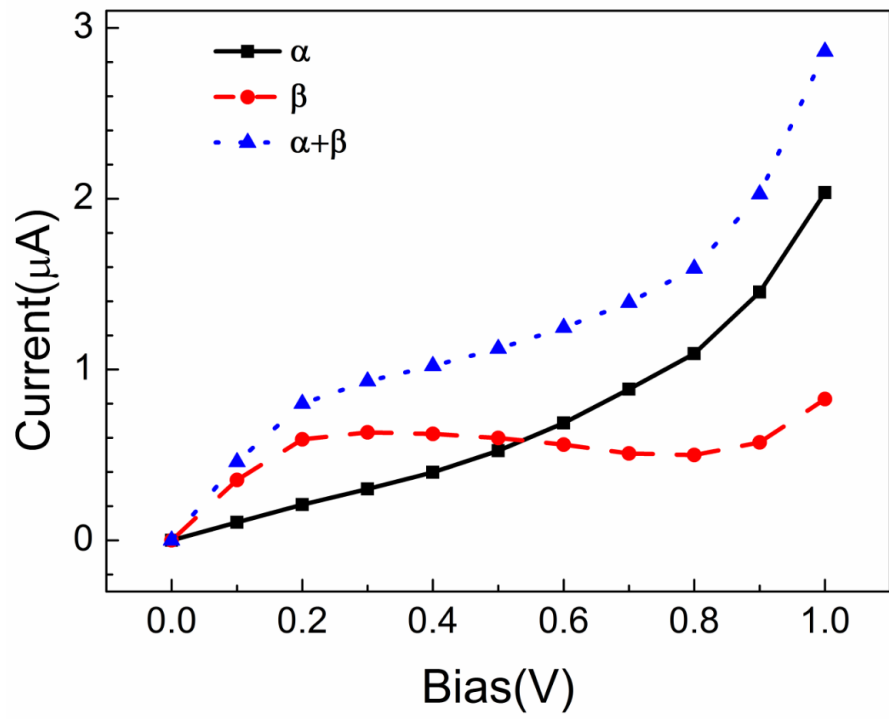


Fig. S1. Spin polarized  $I$ - $V$  curves for device C2.

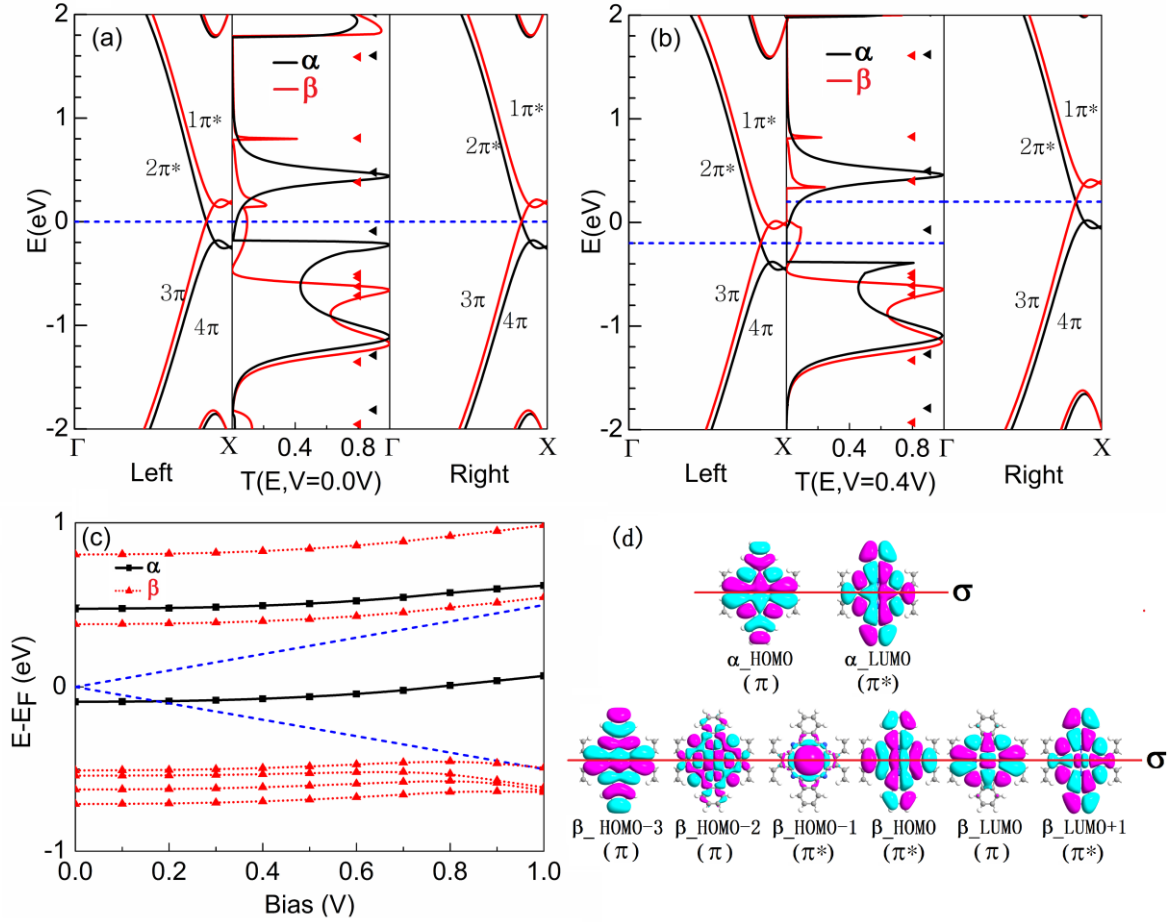


Fig. S2. (a, b) Spin polarized transmission spectra and band structures of both electrodes for C2 at 0 V and 0.4 V. The black and red triangle symbols point to the eigenvalues of spin-up and spin-down frontier molecular orbitals, respectively. (c) Evolution of spin polarized MPSH eigenvalues under bias voltages for C2. (d) Spatial distribution of frontier orbitals for C2.

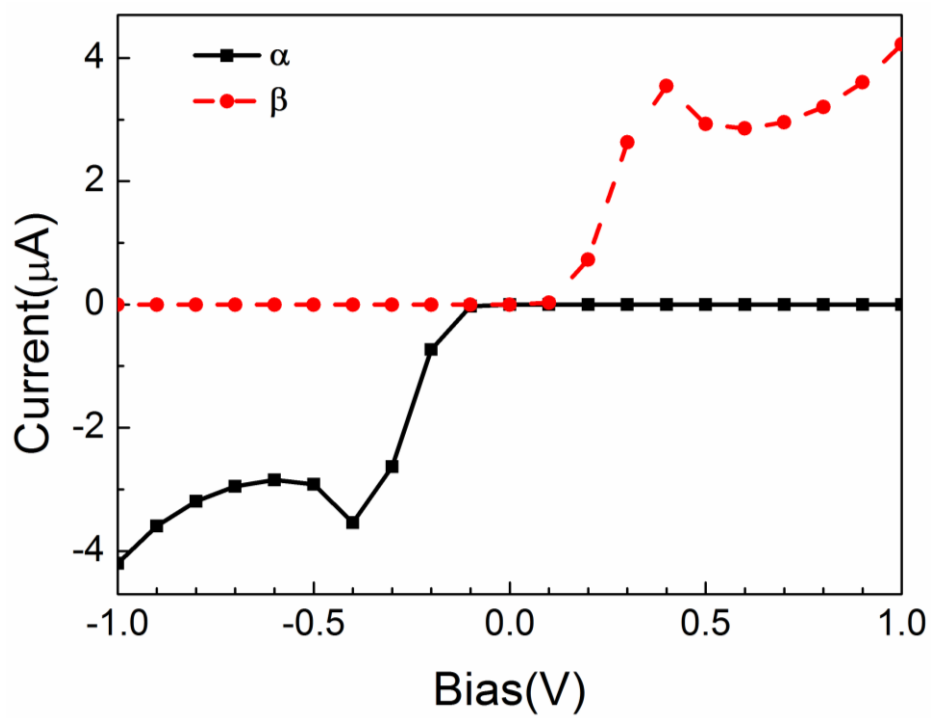


Fig. S3. Spin polarized *I-V* curves for Pc device, in which the two electrodes are antiparallely spin polarized.

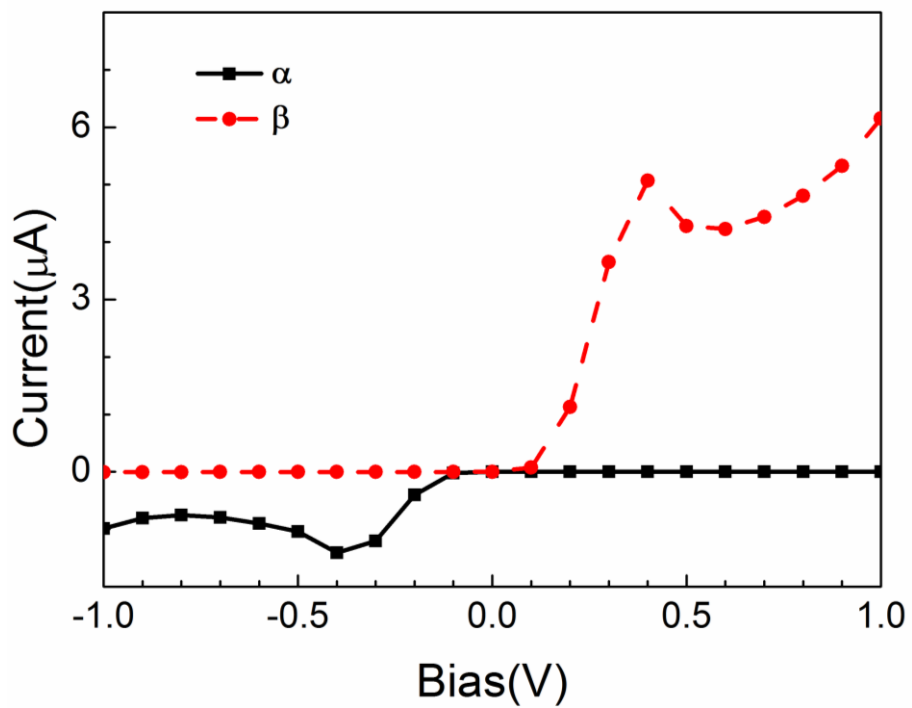


Fig. S4. Spin polarized *I-V* curves for CrPc-based device, in which the two electrodes are antiparallely spin polarized.