Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Design of multifunctional spin logic gates based on manganese porphyrin molecules connected to graphene electrodes

Wenfei Zhang, Guang-Ping Zhang, Zong-Liang Li, Xiao-Xiao Fu, Chuan-Kui Wang, Minglang Wang**

School of Physics and Electronics, Shandong Normal University, Jinan 250358, China

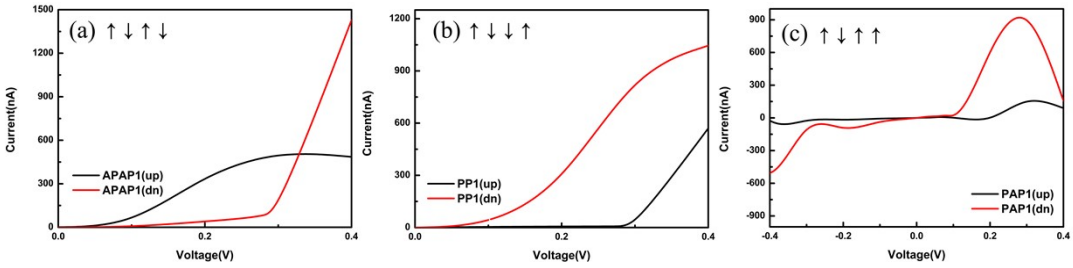

Fig. S1. Spin-resolved I-V curves for three different initial spin configurations named (a) APAP1, (b) PP1, and (c) PAP1. Black line represents the spin-up current and red line represents the spin-down current.

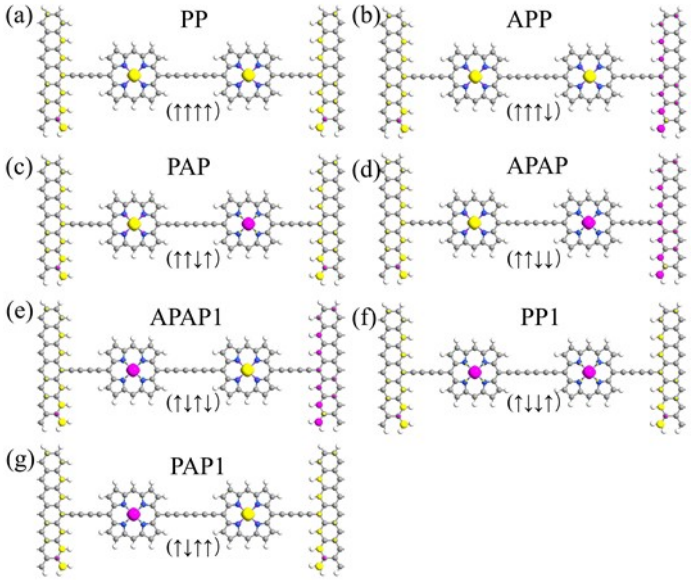

Fig. S2. Distributions of the spin electron density defined as spin up minus spin down for (a) PP,

(b) APP, (c) PAP, (d) APAP, (e) APAP1, (f) PP1 and (g) PAP1.

configuration	Input 1	Input 2	Output	Logic gate	Bias region
(a) PP (↑ ↑ ↑ ↑) APP (↑ ↑ ↑ ↓) PAP1 (↑ ↓ ↑ ↑) APAP1(↑ ↓ ↑ ↓)	1	1	0	NOR	(0.1, 0.3]
	1	0	0		
	0	1	0		
	0	0	1		
(b) PP (↑ ↑ ↑ ↑) PAP (↑ ↑ ↓ ↑) AP1P (↓ ↑ ↑ ↑) AP1AP (↓ ↑ ↓ ↑)	1	1	0	NOR	(-0.1, -0.3]
	1	0	0		
	0	1	0		
	0	0	1		

Fig. S3. Designed spin logical NOR gates under the conditions of corresponding initial spin configurations, truth tables and bias region.

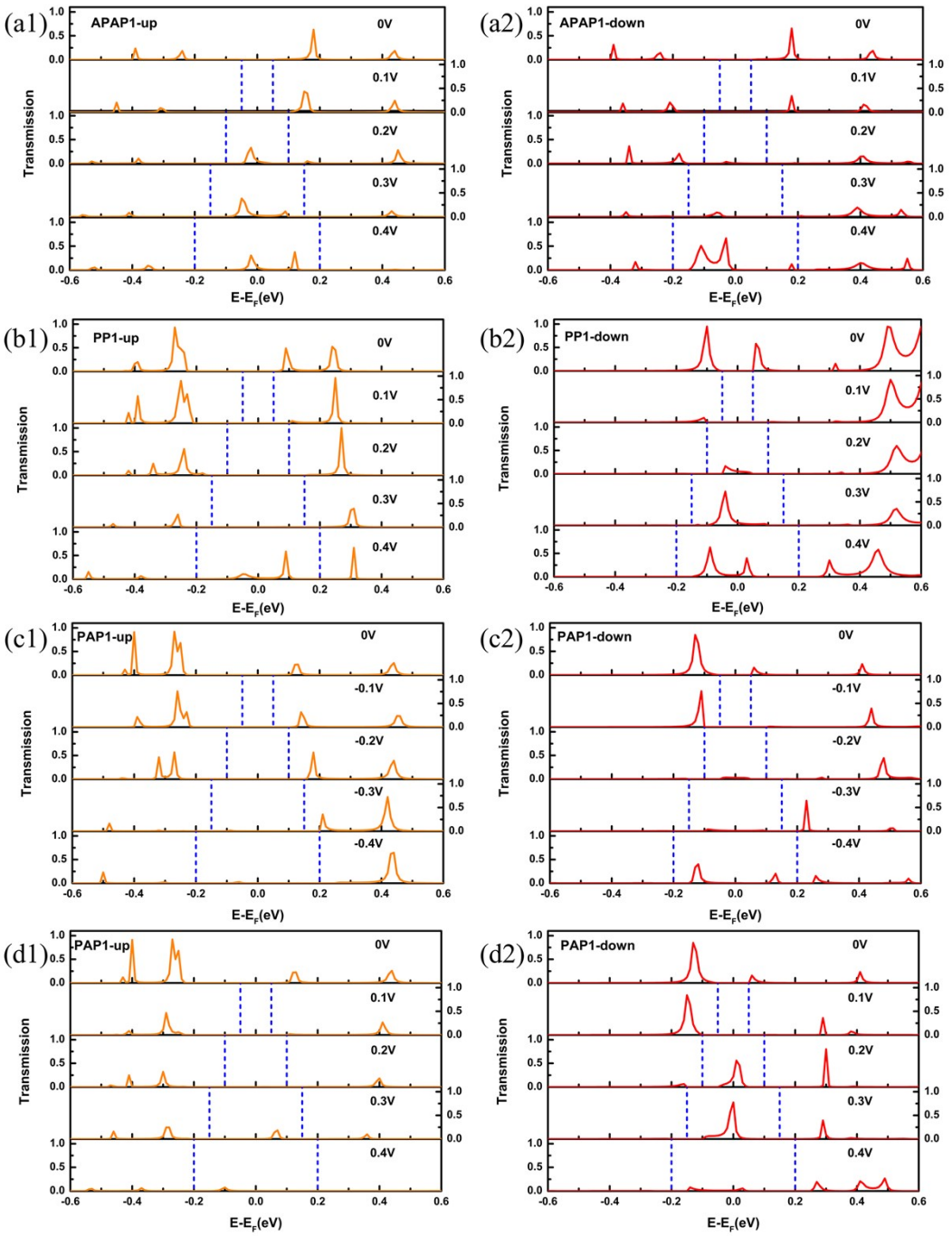

Fig. S4. Spin-resolved transmission spectra respond to the bias voltage for (a) APAP1, (b) PP1, and (c, d) PAP1.

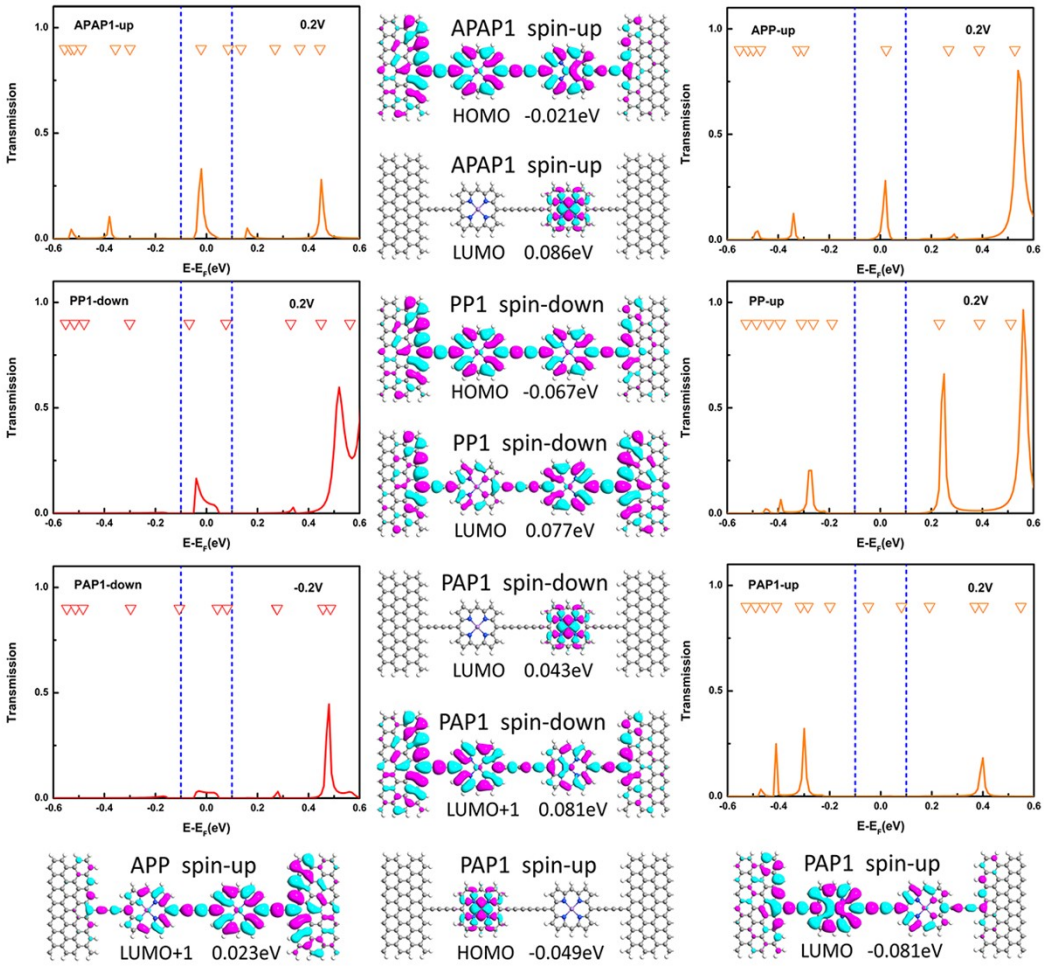

Fig. S5. Spin-resolved transmission spectra, the eigenvalues and corresponding eigenstates of MPSH for APAP1, PP1, PAP1, APP, and PP at -0.2V or 0.2V, where the threshold value of eigenstates is set to 0.02 au.

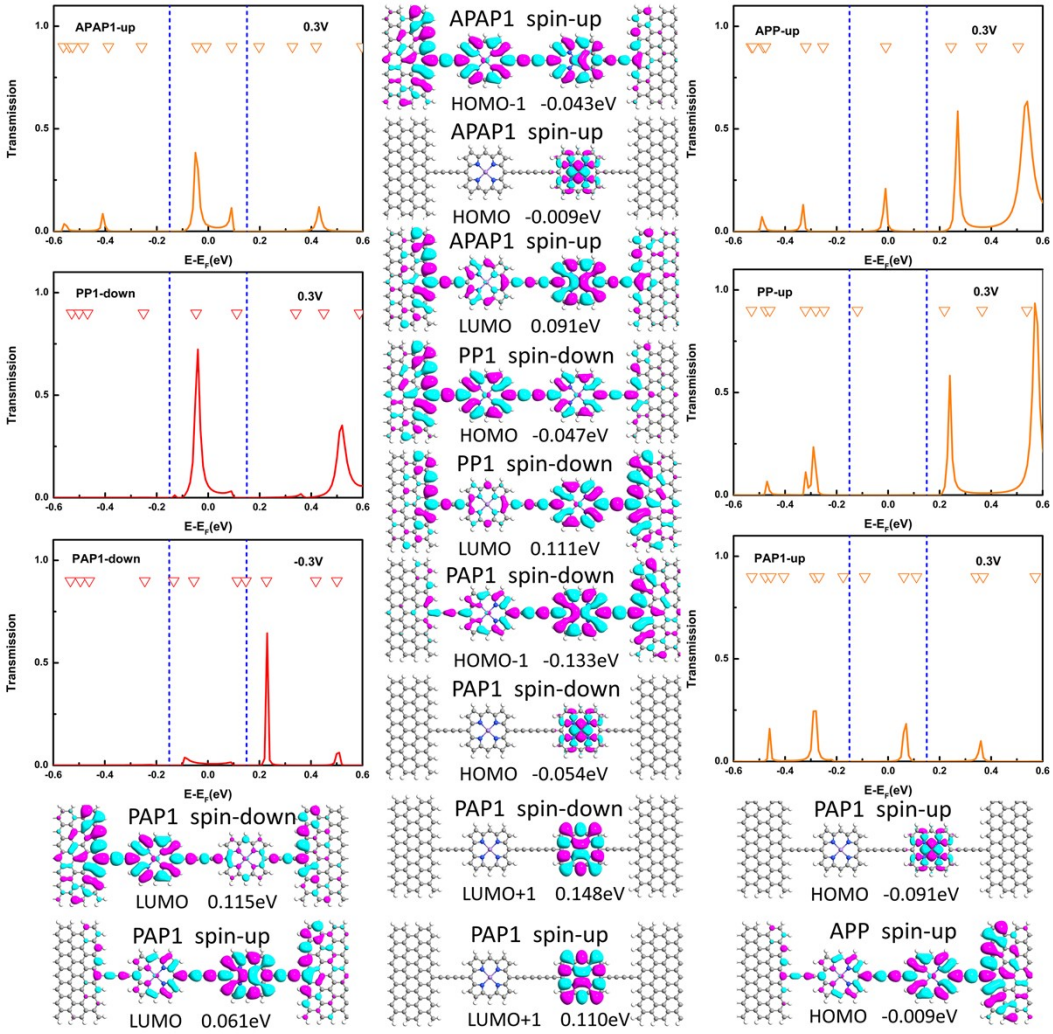

Fig. S6. Spin-resolved transmission spectra, the eigenvalues and corresponding eigenstates of MPSH for APAP1, PP1, PAP1, APP, and PP at -0.3V or 0.3V, where the threshold value of eigenstates is set to 0.02 au.