Supporting Information For the Article in Journal of Materials Chemistry C:

Spin filtering, Magnetic and Electronic Switching Behaviors in Manganese Porphyrin-based Spintronic Device

Jing Zeng and Ke-Qiu Chen[a]

Key Laboratory for Micro-Nano Optoelectronic Devices of Ministry of Education and Department of Applied Physics, Hunan University, Changsha 410082, China

[a]Corresponding authors. E-mail address: keqiuchen@hnu.edu.cn

1. I-V curve for M1 and M2 in the AP spin configurations

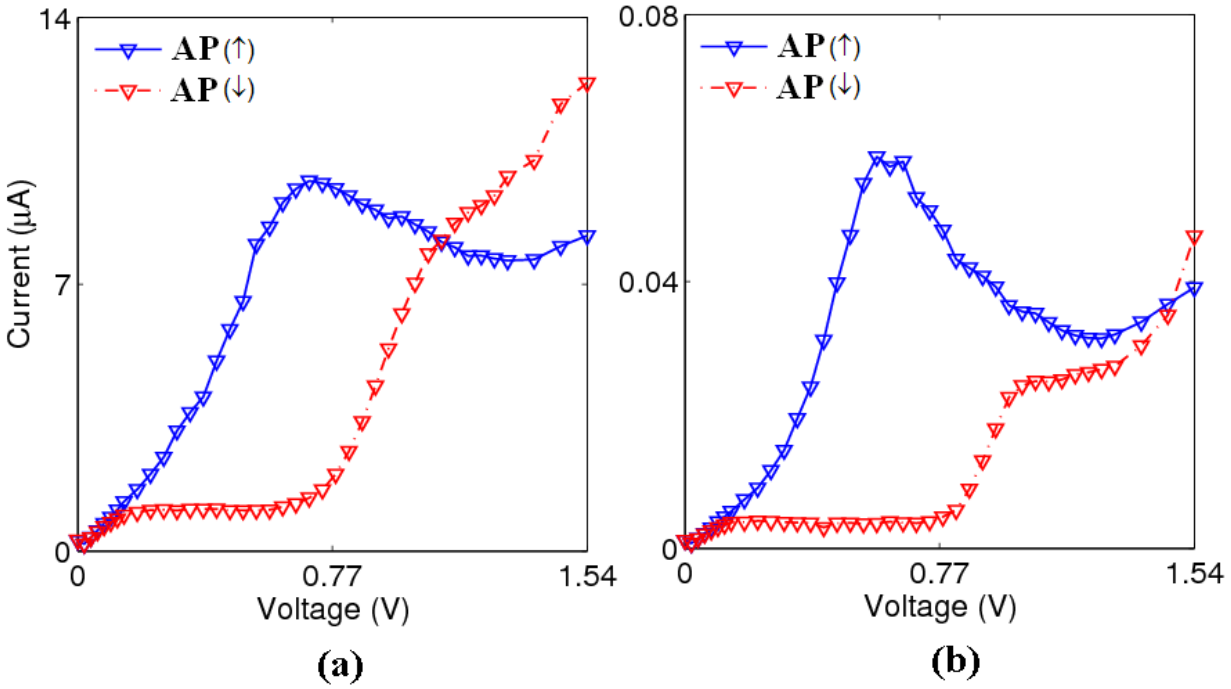

Figure S1. (Color online) (a) [(b)]: calculated current as a function of the applied bias for M1 [M2] in the AP spin configurations.

2. PDOSs for M1

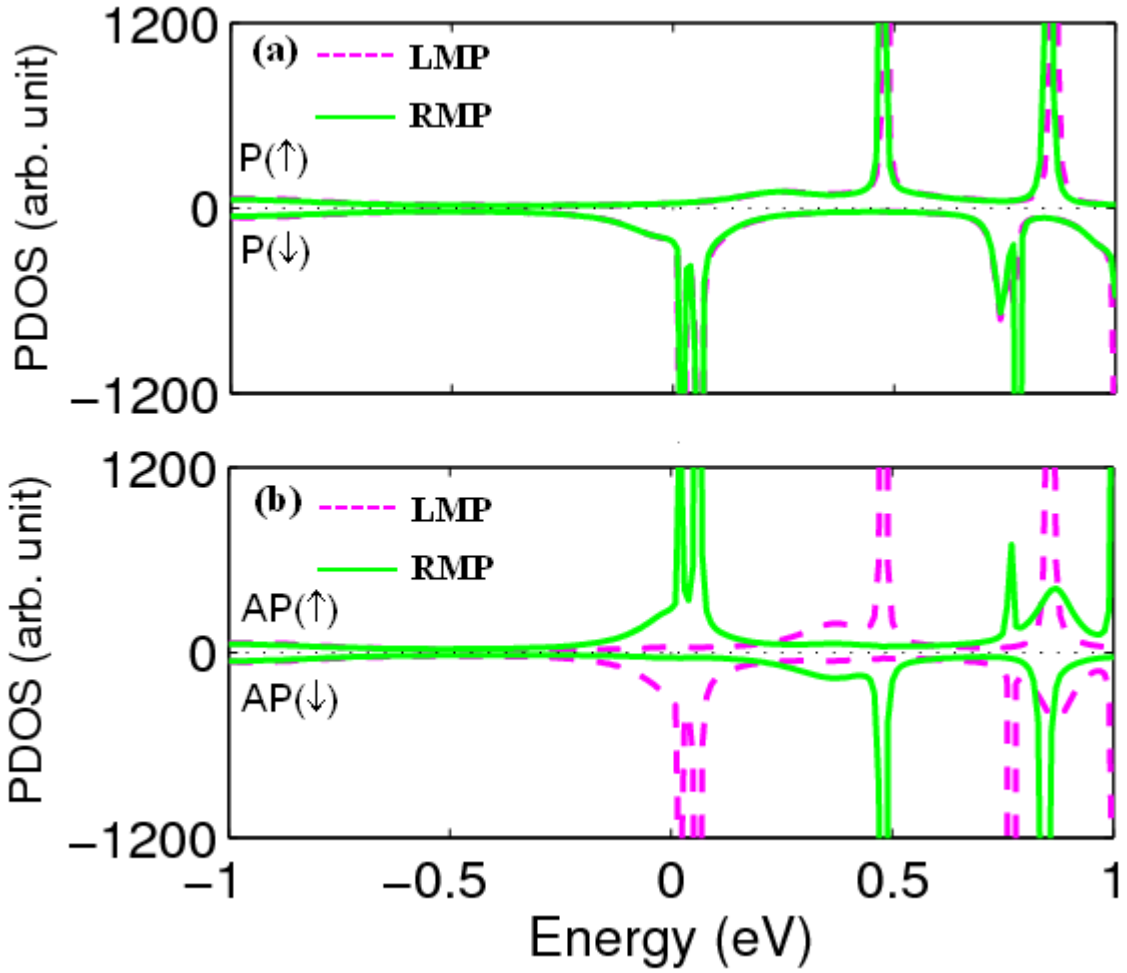

Figure S2. (Color online) PDOSs for the P and AP spin configurations of left manganese porphyrin (LMP) and right manganese porphyrin (RMP) of M1 at zero bias.

When the M1 is set in the P spin configuration, we can find from Fig. S2(a) that for the spin-up state, the electronic states for both LMP and RMP are located far away from the Fermi level. However, for the spin-down state, the PDOSs peaks for both LMP and RMP are located near the Fermi level. Such a distribution characteristics will no doubt lead to the appearance of the spin filtering effect. In the AP spin configuration, it can be seen that, for both spin-up and spin-down states in the energy range [-0.5, 0.5 eV], wherever RMP present PDOS peaks, the LMP would be PDOS valleys, and vice versa. Thus, the spin filtering effect disappear. Furthermore, it is noted from the Fig. 3(a) that for P spin configuration, there is a high spin-down transmission peak lying near the Fermi level, and thus it can contribute to obvious current at the very low bias, leading to low resistance for the system. But for AP spin configuration, the transmission

coefficients are relatively low near the Fermi level due to the mismatch of electronic states of LMP and RMP [see Fig. 3(b) and Fig. S2(b)], which induces high resistance in the system. As a result, the magnetoresistance effect occurs in M1.