Electronic Supplementary Information (ESI) for nanoscale

Supporting Information

Coherent transport through spin-crossover magnet Fe_2

Jing Huang[*,a,b], Rong Xie[a], Weiyi Wang[b], Qunxiang Li[*,b,c] and Jinlong Yang[b,c]

[a]*School of Materials and Chemical Engineering, Anhui Jianzhu University, Hefei, Anhui 230601, China. E-mail: jhuang@ustc.edu.cn*
[b]*Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, Anhui 230026, China. E-mail: liqun@ustc.edu.cn*
[c]*Synergetic Innovation Center of Quantum Information and Quantum Physics, University of Science and Technology of China, Hefei, Anhui 230026, China*

Figure S1 shows the spin density of the isolated SCO magnets Fe_2 complexes and the corresponding junctions with the [HS-HS] and [HS-LS] configurations.

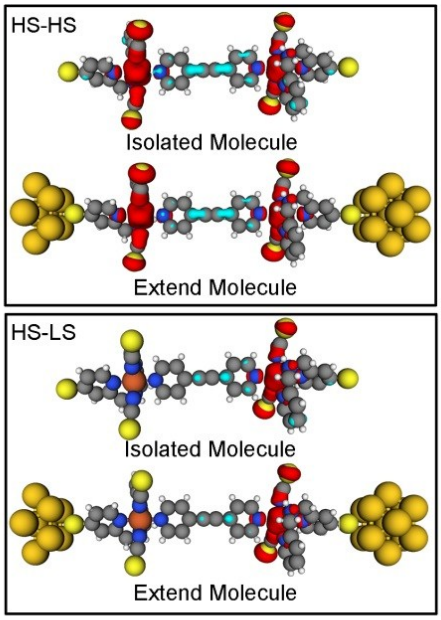

Fig. S1 Spin density of the isolated SCO magnets Fe_2 complexes and the corresponding junctions.

Figure S2 shows the zero-bias transmission curves of the SCO magnets Fe_2 complexes with the [HS-HS] and [LS-LS] configurations connecting to gold electrodes via both thiol and thiocyanato end groups.

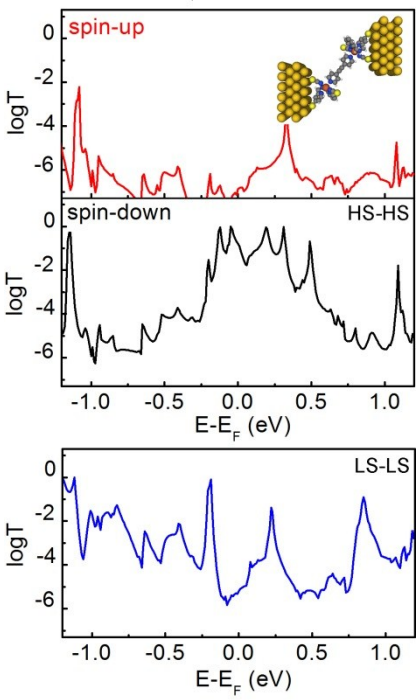

Fig. S2 Transmission curves of the SCO magnets Fe_2 sandwiched between two Au(100) electrodes via both thiol and thiocyanato end groups.

Figure S3 shows the zero-bias transmission curves of the SCO magnets Fe_2 with the [HS-HS] and [LS-LS] configurations sandwiched between two periodic Au(111) electrodes, which are modeled with 6×6 supercells.

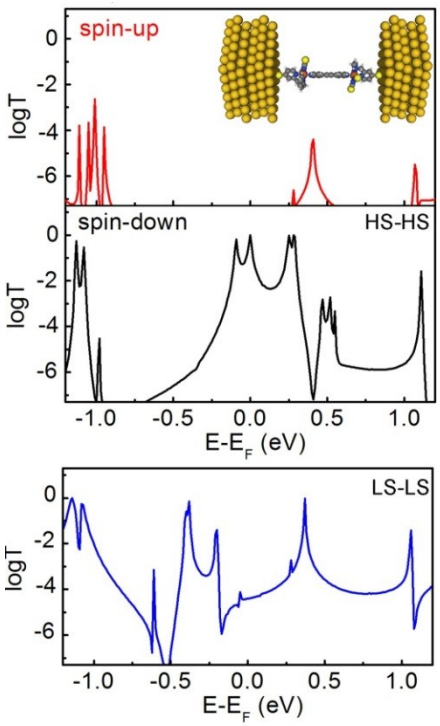

Fig. S3 Transmission curves through the SCO magnets Fe_2 sandwiched between two periodic Au(111) electrodes

Figure S4 shows the zero-bias transmission curves of two SCO magnets Fe_2 sandwiched between two periodic Au(100) electrodes, which are modeled with 8×8 supercells.

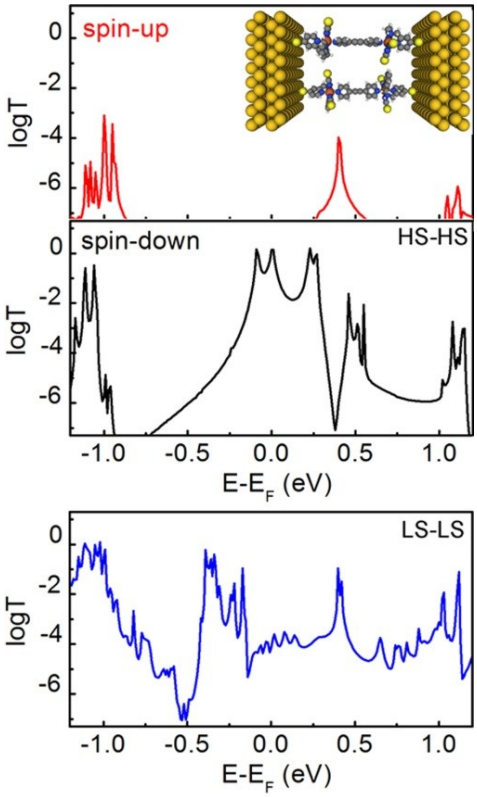

Fig. S4 Transmission curves of two SCO magnets Fe_2 sandwiched between two periodic Au(100) electrodes

Figure S5 shows the 3d partial density of states (PDOS) for the HS Fe(II) cation in the isolated SCO

magnets Fe_2 as well as its $3d^6$ electron occupations.

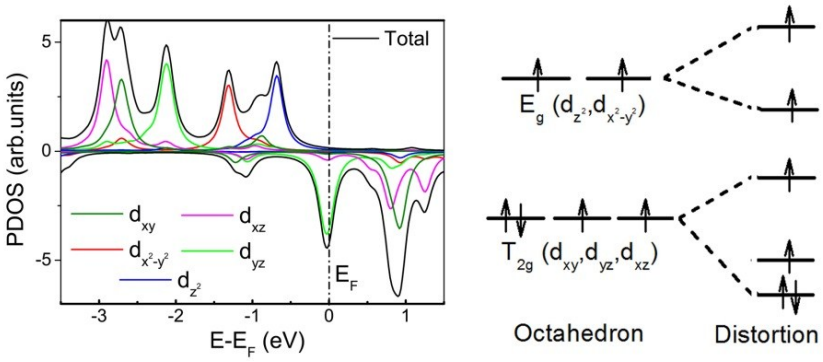

Fig. S5 PDOS and electron configuration of the HS Fe(II) cation in the SCO magnets Fe_2.

Figure S6 shows the bias-dependent transmission curves of the SCO magnets Fe_2 with the [LS-LS] configuration.

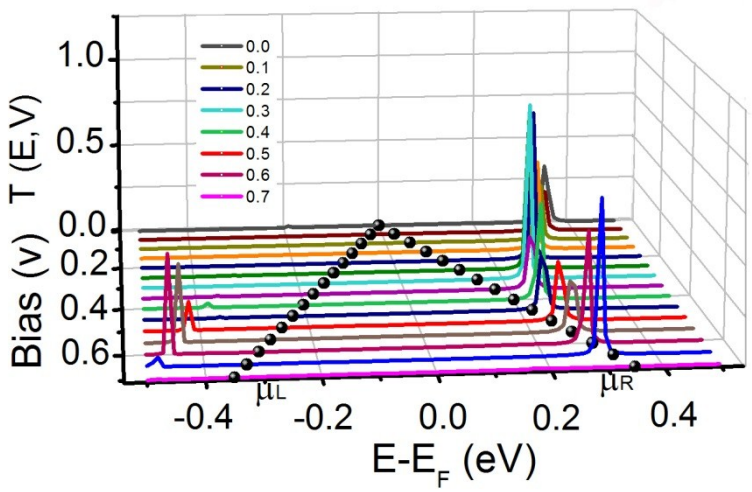

Fig. S6 Bias-dependent transmission curves of the SCO magnets Fe_2 with the [LS-LS] configuration.

Fig. S7 shows the bias-dependent transmission curves of the SCO magnets Fe_2 with the [LS-HS] configuration for the spin-down electrons.

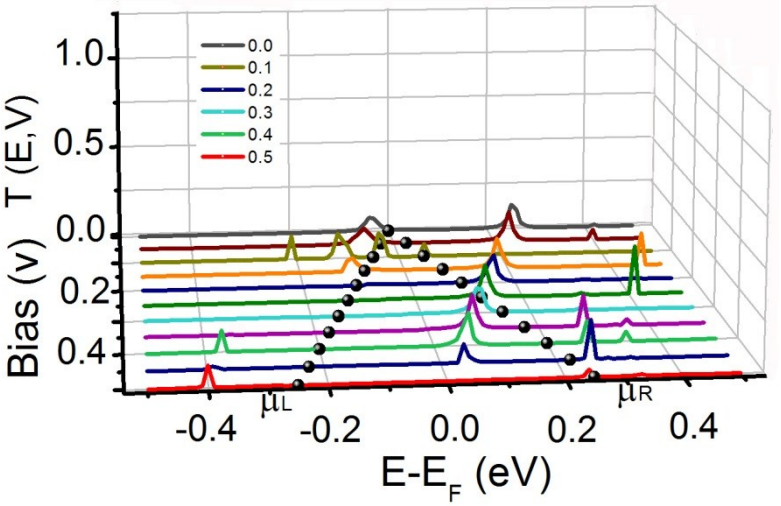

Fig. S7 Bias-dependent transmission curves of the spin-down electrons for the SCO magnets Fe_2 with the [LS-HS] configuration.