magnetochemistry

Supplementary Materials: Investigation of a Tetrathiafulvalene-Based Fe^{2+} Thermal Spin Crossover Assembled on Gold Surface

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1. XPS

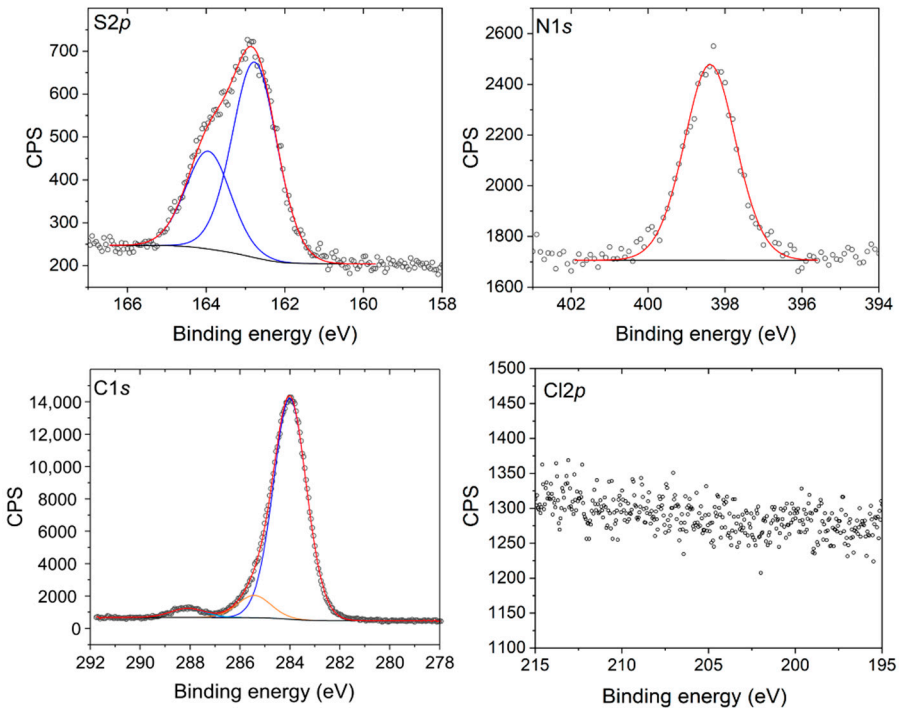

Figure S1. S2*p*, N1*s*, C1*s* *and* Cl2*p* regions of XPS spectra of [$Fe(H_2Bpz_2)_2$(**L**)] thick film on Au.

Table S1. Component used for fitting Fe2*p* XPS spectra of [Fe(H_2Bpz_2)$_2$(**L**)] thick film on Au.

T	**Fe$_{A+A'}$** *B.E. (ΔEso)*	**Fe$_{B+B'}$** *B.E. (ΔEso)*	**Fe$_{C+C'}$** *B.E. (ΔEso)*	**Fe$_{D+D'}$** *B.E. (ΔEso)*	**Fe$_{E+E'}$** *B.E. (ΔEso)*
Room temperature	710.2 eV (13.1 eV)	711.9 eV (13.5 eV)	713.7 eV (13.5 eV)	715.9 eV (13.2 eV)	718 eV (13.1 eV)
140 K	710.1 eV (12.9 eV)	712 eV (13.4 eV)	713.8 eV (13.5 eV)	716 eV (13.1 eV)	717.9 eV (13.1 eV)

Table S2. Semi-quantitative analysis of [Fe(H_2Bpz_2)$_2$(**L**)] thick film and of [Fe(H_2Bpz_2)$_2$(**L**)]@Au(111).

Sample	**S2*p* [%]**	**N1*s* [%]**	**Fe2*p* [%]**
Expected Stoichiometry	31.6	63.2	5.3
Monolayer	47.1 ± 2.3	39.3 ± 2.0	13.6 ± 0.7
Thick film	35.5 ± 1.8	60.6 ± 3.0	4.0 ± 0.2

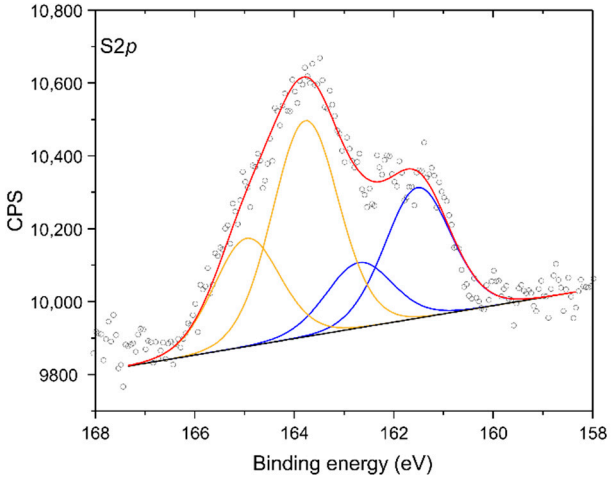

Figure S2. S2*p* region of XPS spectra of [Fe(H_2Bpz_2)$_2$(**L**)] monolayer on Au. Blue components are attributable to sulfur atoms bound to gold substrate.

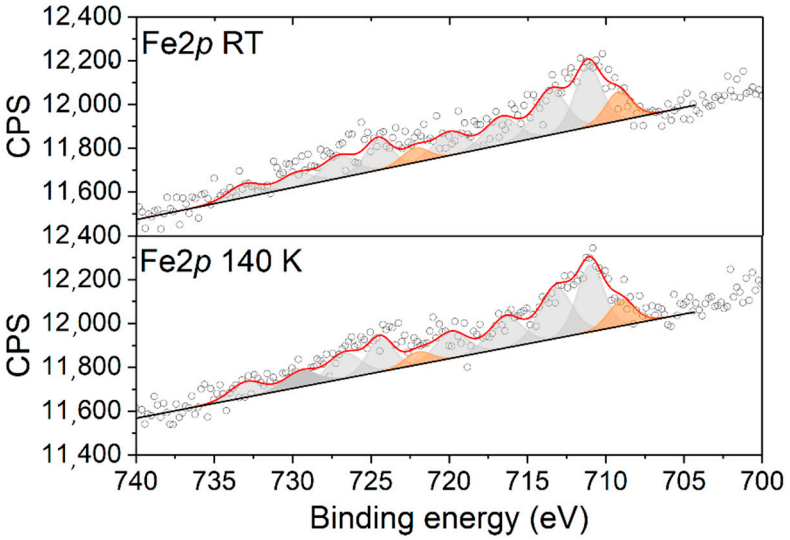

Figure S3. Fe2*p* region of XPS spectra of [Fe(H_2Bpz_2)$_2$(**L**)]@Au(111) at room temperature and at 140 K.

2. XAS

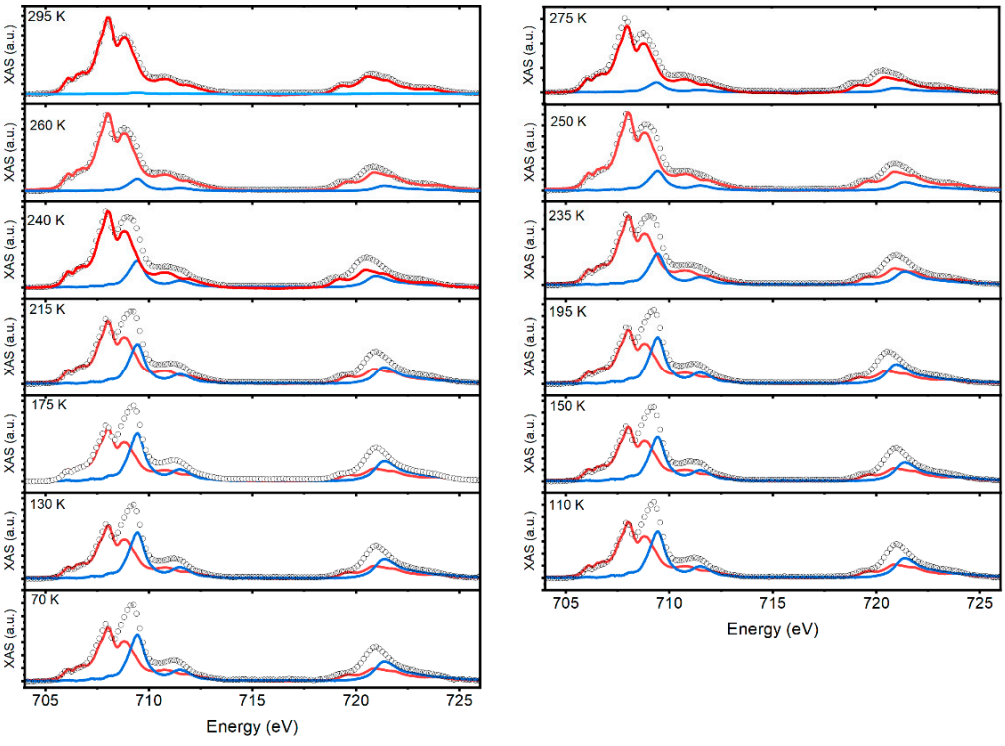

Figure S4. XAS spectra at the Fe $L_{2,3}$ edge of [Fe(H_2Bpz_2)$_2$(**L**)] thick film between 295 K and 70 K. Experimental spectra (dots), HS contribution (red line) and LS contribution (blue line).

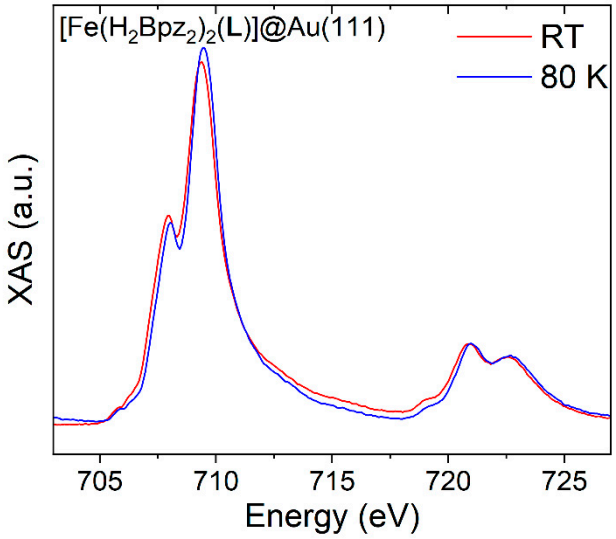

Figure S5. XAS spectra at the Fe $L_{2,3}$ edge of [Fe(H_2Bpz$_2$)$_2$(**L**)]@Au(111) at 80 K and 295 K.