
Electronic supplementary information

Room Temperature Control of Spin States in a Thin Film of a Photochromic Iron(II) Complex

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S1. Additional ToF-SIMS characterization

Table S1. Summary of ToF-SIMS peaks expected and experimentally found for bulk and evaporated sample.

	Theoretical (m/z)	Evaporated (m/z.)	Intensity	Bulk (m/z)	Intensity
[M-pz] ⁺	683.19	683.1	vw	683.1	w
[M-Bpz] ⁺	669.17	669.11	w	669.11	s
[M-B(pz) ₂] ⁺	603.13	603.08	s	603.08	s
[M-B(pz) ₂ -Bpz] ⁺	523.07	523.02	s	523.02	s
[M-2B(pz) ₂]	457.05	457.06	m	457.01	m
[M-2B(pz) ₂ -Fe] ⁺	401.11	401.12	m	401.09	m

pz = *H*-pyrazole

Bpz = 1-boryl-1*H*-pyrazole

B(pz)₂ = di(1*H*-pyrazol-1-yl)borane

S2. AFM Characterization

Morphological analysis has been carried out with a NT-MDT Solver P47pro Scanning Probe Microscope (NT-MDT, Zelenograd, Moscow, Russia; www.ntmdt.ru) equipped with NGS01 NT-MDT. The image analysis has been carried out with Gwyddion software.^{S1} AFM images were taken in tapping mode in air. The estimated thickness was about 16.8 nm, and the measured one it's about 15 nm (Fig. S1a). A nominal 5nm molecular film on Au (111) it's shown in Fig. S2b). Imaging showed a nice defect-free SCO deposit without the presence of pin-hole on the surface.

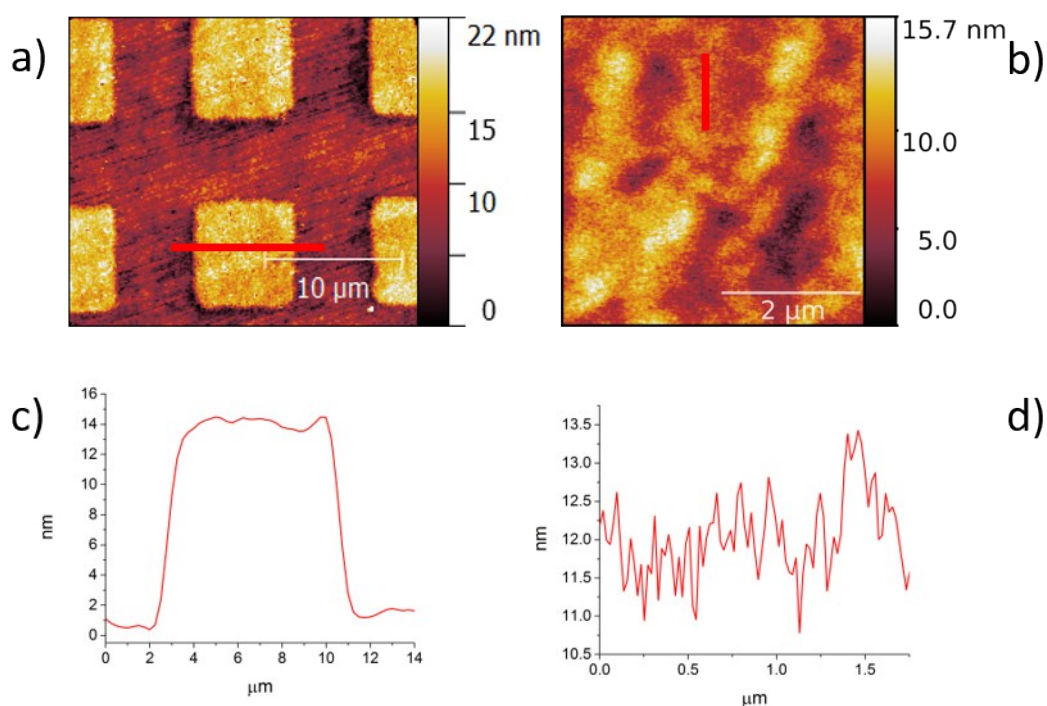


Figure S1. a) AFM image (25X25 μm) of patterned molecular film obtained via shadow masking technique on SiO_x surface; b) image (15X15 μm) of molecular film on Au(111), c) Topography profile of patterned molecular film along the red line in figure a); d) topography profile of molecular film on Au (111) along the red line in b).

S3. Magnetic characterization of the sublimated film

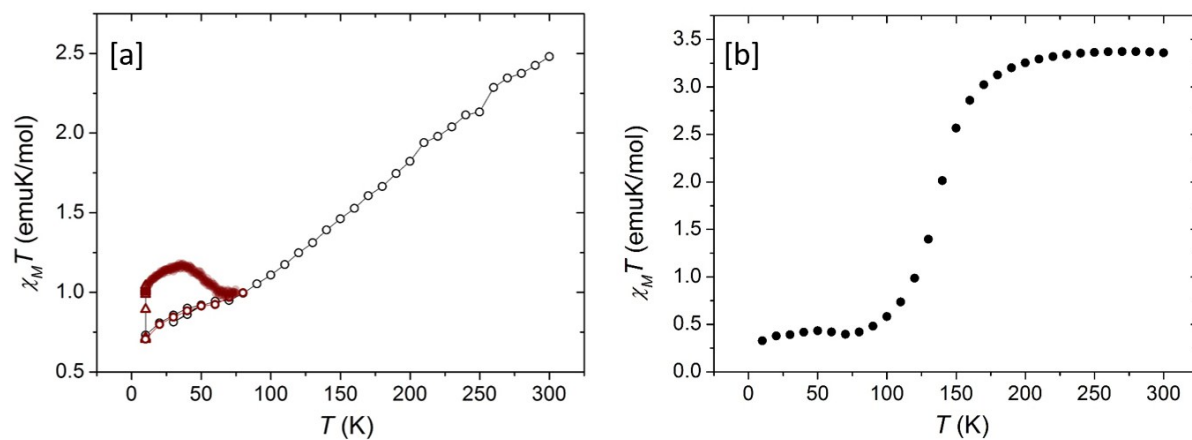


Figure S2. [a] Temperature dependence of the $\chi_M T$ product for a 200 nm film of **1** before (empty black dots and empty red dots), during (empty red triangles) and after (full red dots) 532 nm laser light irradiation at 10 K; [b] Temperature dependence of the $\chi_M T$ product for a polycrystalline sample of **1**.

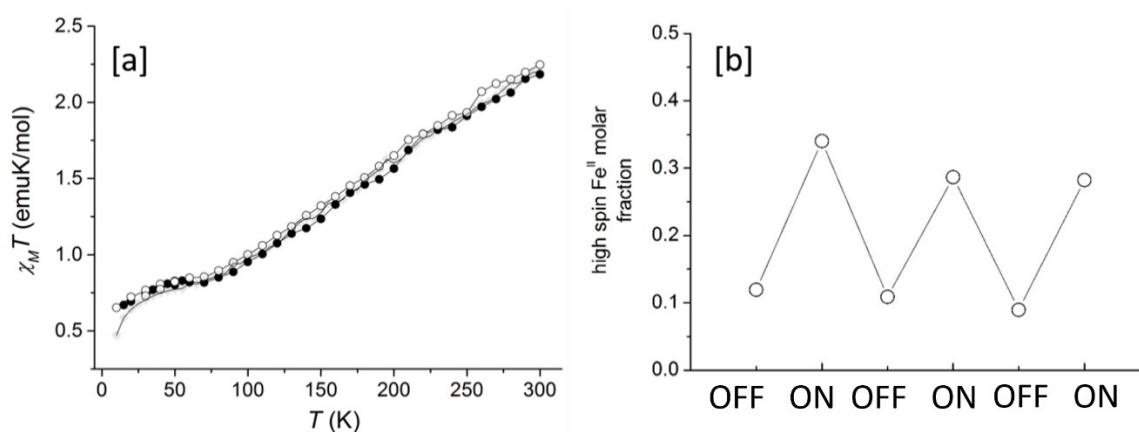
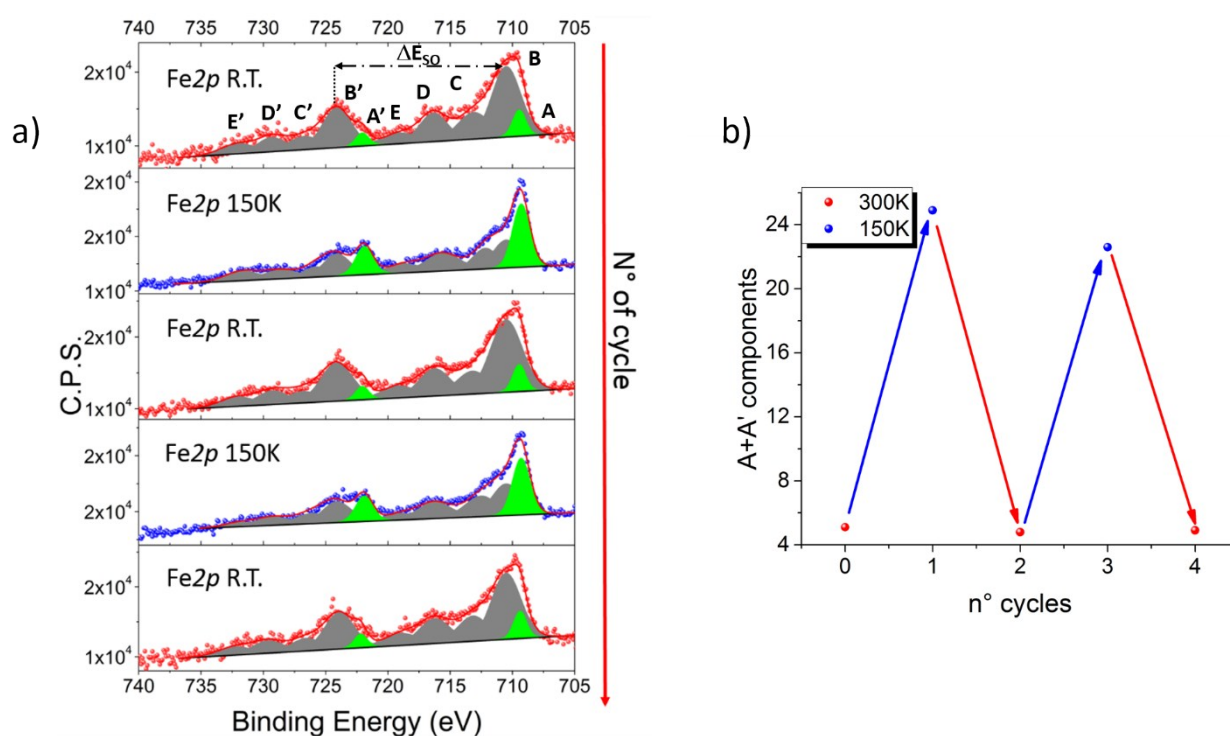


Figure S3. [a] Temperature dependence of the $\chi_M T$ product for a 200 nm film of **1**, before (full dots) and after (empty dots and fading grey lozenges) UV irradiation ($\lambda = 282$ nm); [b] Reversibility of the optically induced SCO interconversion (LIESST effect, $\lambda = 532$ nm) at low temperature for a 200 nm film of **1**.

S4. Additional XPS-UPS characterization

Table S2. Theoretical and XPS estimated atomic percentages and ratios for a SCO thin film (5.3 nm) evaporated on Au(111).

	Fe 2p	N 1s	S 2p	B 1s	C 1s
Exp. %	1.8	18.7	3.0	3.8	72.7
Theor. %	1.5	15.5	3.1	3.1	76.9



	300 K		150 K		300 K		150 K		300 K	
	%	B.E. (ΔE S.O.)	%	B.E. (ΔE S.O.)	%	B.E. (ΔE S.O.)	%	B.E. (ΔE S.O.)	%	B.E. (ΔE S.O.)
A+A'	5.10	709.26 eV (12.4 eV)	24.90	709.24 eV (12.4)	4.80	709.20 eV (12.4 eV)	22.60	709.25 eV (12.4 eV)	4.91	709.12 eV (12.4 eV)
B+B'	46.70	710.51 eV (13.4 eV)	32.60	710.30 eV (13.4 eV)	47.40	710.30 eV (13.4 eV)	35.20	710.30 eV (13.4 eV)	47.2	710.30 eV (13.4 eV)
C+C'	20.20	712.88 eV (13.4 eV)	18.30	712.31 eV (13.4 eV)	19.90	712.72 eV (13.4 eV)	19.80	712.49 eV (13.4 eV)	19.9	712.80 eV (13.4 eV)
D+D'	19.10	715.94 eV (13.4 eV)	14.80	715.60 eV (13.4 eV)	18.10	715.86 eV (13.4 eV)	14.10	715.81 eV (13.4 eV)	16.9	715.9 eV (13.4 eV)
E+E'	8.90	718.43 eV (13.4 eV)	9.40	718.30 eV (13.4 eV)	9.80	718.44 eV (13.4 eV)	8.30	718.3 eV (13.4 eV)	11.1	712.45 eV (13.4 eV)

Figure S4. a) Additional reversible temperature switching of **1** complex in a 5.3 nm thick film in the Fe2p region; b) Percentage of green component in function of the number of thermal cycles; Table with the percentage of all the component of the fitting procedure.

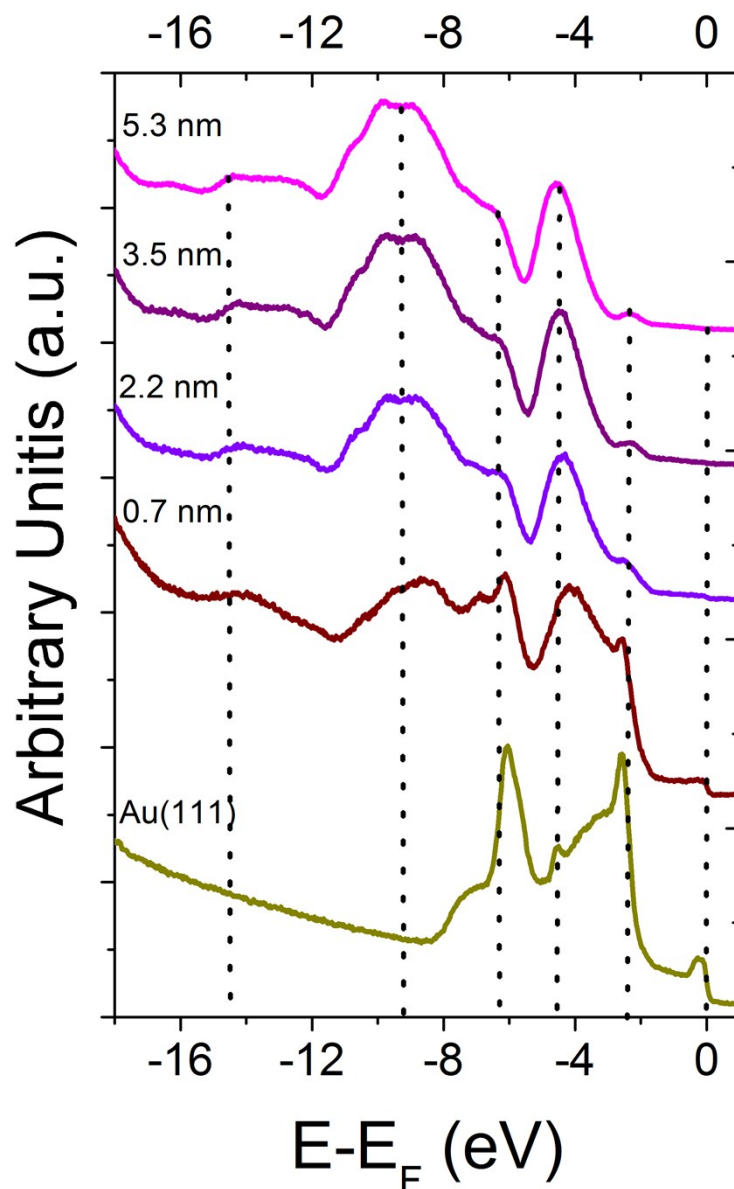


Figure S5. UPS spectra from -18 eV to 1 eV ($E-E_F$) at R.T from 0.7 nm to 5.3 nm in nominal thickness of **1**.

S5. Calculated TDOS

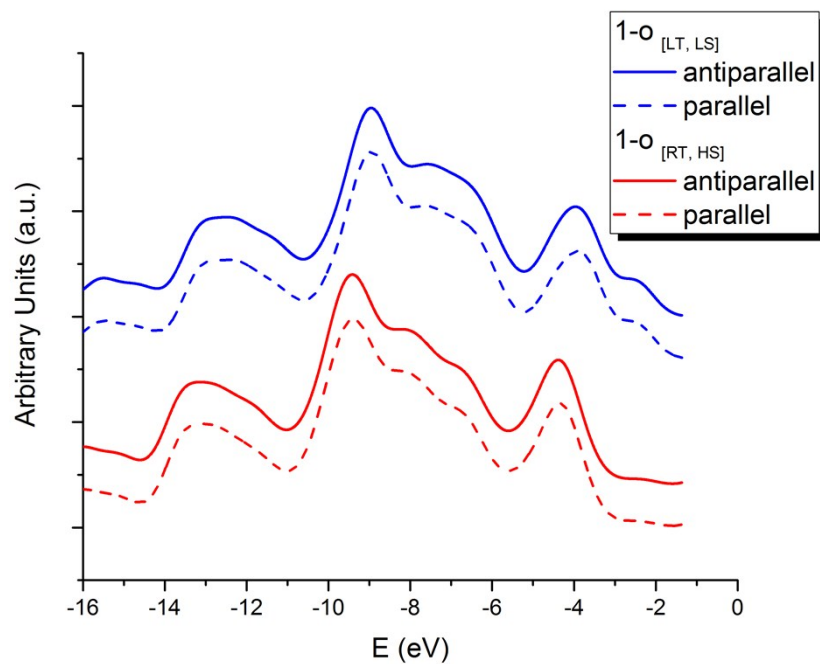


Figure S6. TDOS for parallel and antiparallel conformers in HS and LS states.

References

- S1 David Nečas, Petr Klapetek, Gwyddion: an open-source software for SPM data analysis, *Cent. Eur. J. Phys.* **10**(1) (2012) 181-188