

Supplementary Materials to:

Magnetic field perturbations to a soft X-ray activated Fe (II) molecular spin state transition

Guanhua Hao,^{1,2} Alpha T. N'Diaye,^{2*} Thilini K. Ekanayaka,¹ Ashley S. Dale,³ Xuanyuan Jiang,¹ Esha Mishra,¹ Corbyn Mellinger,¹ Saeed Yazdani,³ John Freeland,⁴ Jian Zhang,⁵ Ruihua Cheng,^{3*} Xiaoshan Xu,¹ Peter A. Dowben^{1*}

¹ Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, NE 68588-0299, U.S.A; guanhua.hao@huskers.unl.edu, thiliniek@huskers.unl.edu, neojxy@gmail.com, emishra@huskers.unl.edu, corbyn.mellinger@huskers.unl.edu, xiaoshan.xu@unl.edu, pdowben1@unl.edu

² Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, U.S.A.; ghao@lbl.gov, atndiaye@lbl.gov

³ Physics Department, Indiana University-Purdue University-Indianapolis, Indianapolis, IN 46202, U.S.A.; daleas@iupui.edu, syazdani@iupui.edu, rucheng@iupui.edu

⁴ Argonne National Laboratory, Advanced Photon Source, Bldg. 431/E003, 9700 South Cass Ave., Argonne IL 60439, U.S.A.; freeland@anl.gov

⁵ Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, U.S.A.; JianZhang@lbl.gov

* Correspondence: pdowben1@unl.edu; Tel.: +1-402-472-9838 (PAD); atndiaye@lbl.gov; Tel.: +1-510-486-5926 (ATN); rucheng@iupui.edu; Tel.: +1-317-274-6902 (RC)

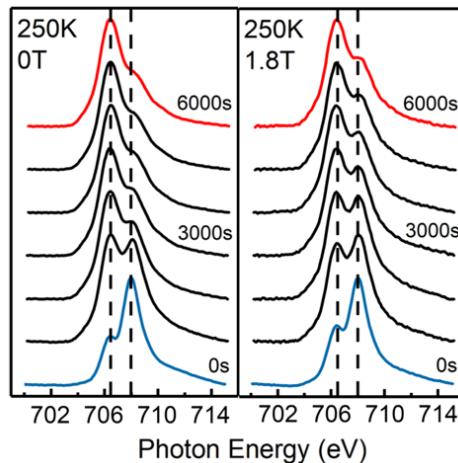


Figure S1. The time evolution of the X-ray absorption spectra with and without an applied 1.8T magnetic field of $[Fe\{H_2B(pz)_2\}_2(bipy)]$, under a constant incident X-ray fluence at 250 K. The spectra in blue are indicative of the low spin state, while the spectra in red are largely indicative of the high spin state.

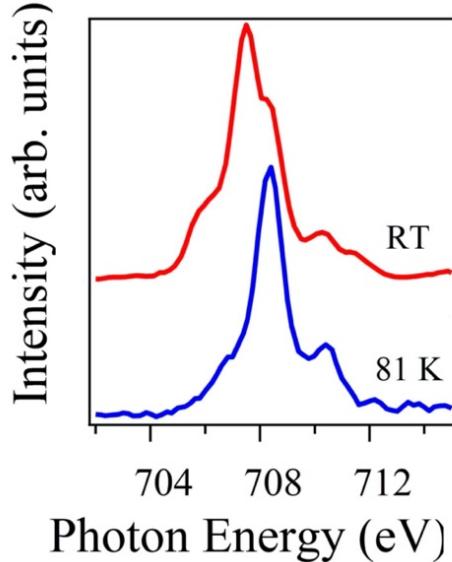


Figure S2. Higher resolution X-ray absorption spectra showing an example of reference spectra for the high spin state and low spin state of $[Fe\{H_2B(pz)_2\}_2(bipy)]$ above and below the accepted spin transition temperature in the region of 160 K. The reference spectra provide a facile mechanism for ascertaining spin state occupancy.

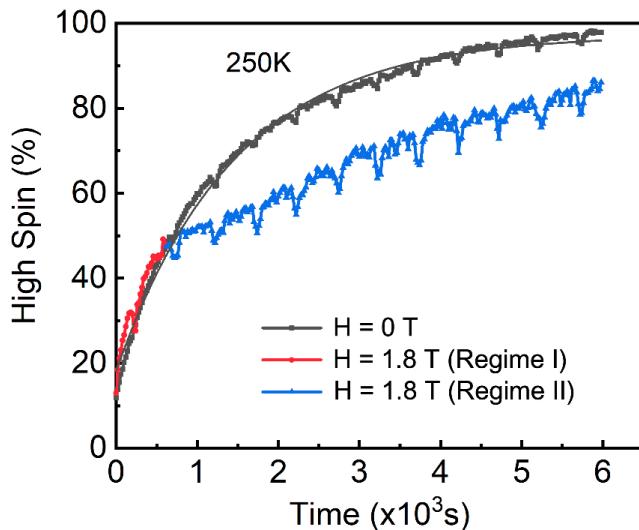


Figure S3. The evolution of the high spin state occupancy in the $[Fe\{H_2B(pz)_2\}_2(bipy)]$ molecular thin film that accompany an incident soft X-ray fluence at 250 K, in the absence of an applied magnetic field (black) as well as in the presence of a 1.8 T applied magnetic field (red and blue). Exponential fit to the high spin state conversion in the field-free case is indicated as a thin solid black line.