

SUPPORTING INFORMATION

Monitoring Spin-Crossover phenomena via Re(I) luminescence in hybrid Fe(II) silica coated nanoparticles

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1.- X-Ray Powder Diffraction Analysis.

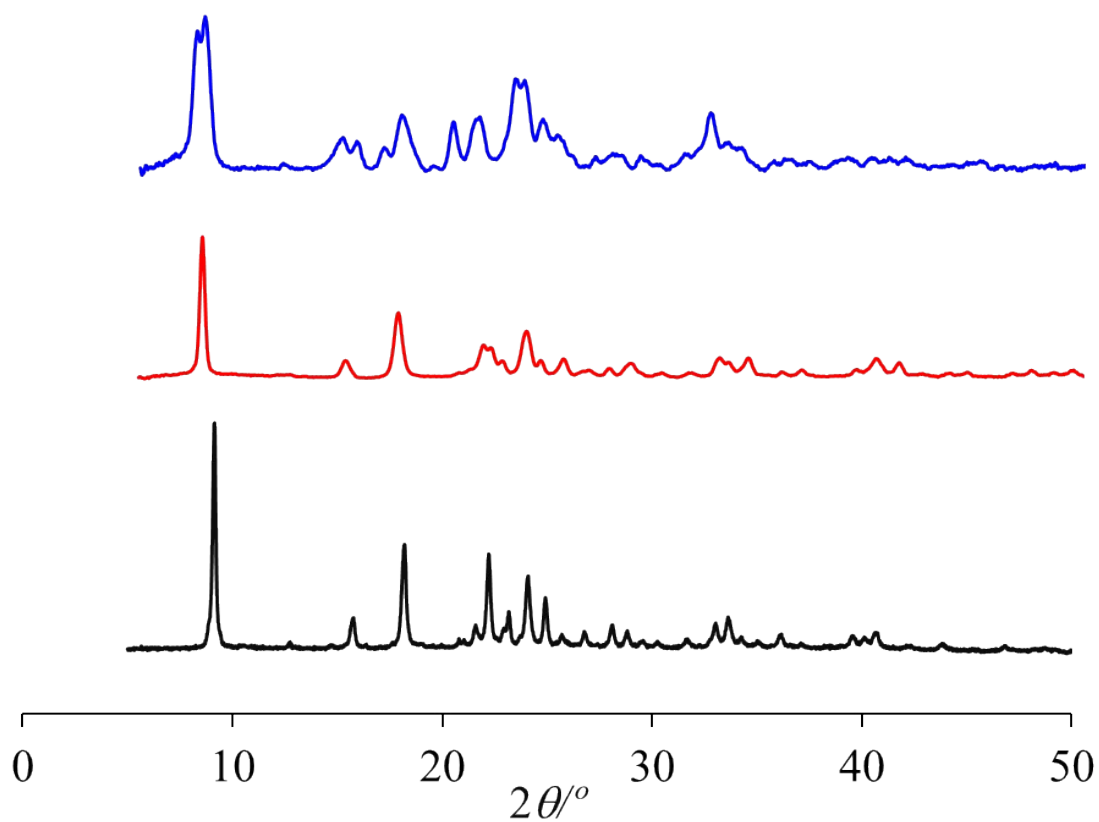


Figure S1. Experimental XRPD diagrams for bulk [Fe(NH₂-Trz)₃](BF₄)₂ polymer (black) and samples **1** (red) and **1@SiO₂** (blue).

2.- Elemental Analysis.

The molecular weights determined by elemental analysis were considered to determine the molar magnetic susceptibility.

Sample		C [%]	N [%]	H [%]	Proposed Formula
1	Found	14.70	33.11	3.17	[Fe(NH ₂ Trz) ₃](BF ₄) ₂ ·H ₂ O
	calcd	14.39	33.60	2.82	MW = 500.08 gmol ⁻¹
1@SiO₂	Found	12.29	28.51	2.87	[Fe(NH ₂ Trz) ₃](BF ₄) ₂ ·(SiO ₂) _{1.5} ·H ₂ O
	calcd	12.20	28.48	2.39	MW = 590.03 gmol ⁻¹
1@SiO₂/Re	Found	14.85	28.79	2.98	-----
	calcd	---	---	---	

Table S1.- Elemental analyses for samples **1**, **1@SiO₂** and **1@SiO₂/Re**.

3.- NMR characterization.

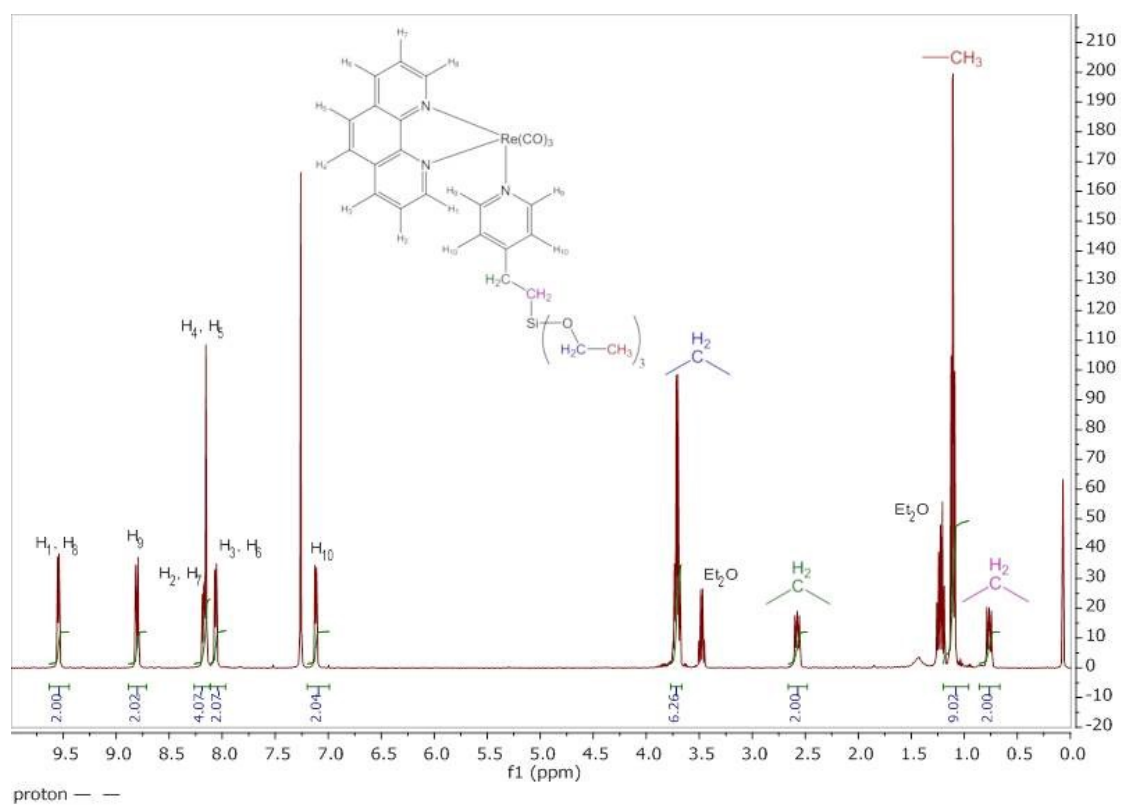


Figure S2.- $^1\text{H-NMR}$ spectrum of **Re** in CD_3Cl .

4.- Kinetics for Time-resolved photoluminescence of Re and 1@SiO₂/Re.

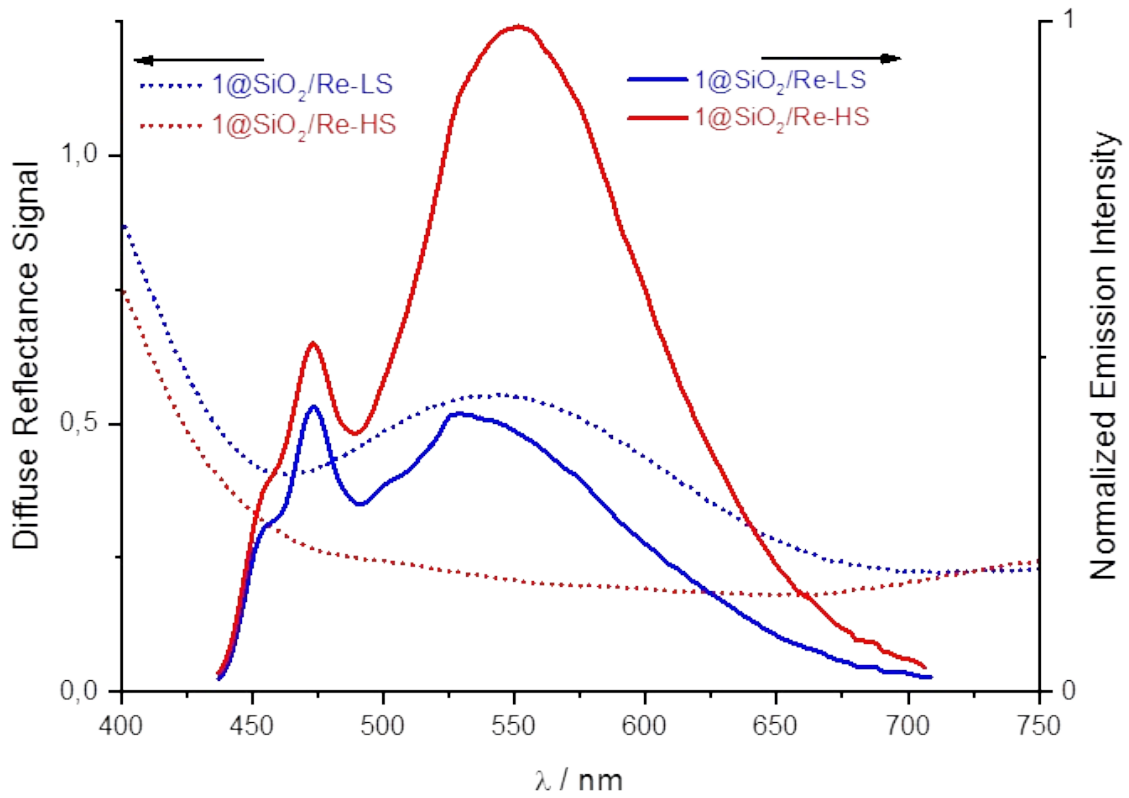


Figure S3.- Diffuse reflectance (dotted lines) and Emission (full lines) spectra of **1@SiO₂/Re** measured at T = 280 K (blue) and T = 330 K (red).

Solid state samples were excited at $\lambda_{exc.} = 350$ nm at two different temperatures, T = 273 K and T = 330 K. Decays were fitted to the two or three-exponential functions:

$$I = A_1 e^{-\frac{t}{\tau_1}} + A_2 e^{-\frac{t}{\tau_2}} + y_0 \quad \text{eq. 1}$$

$$I = A_1 e^{-\frac{t}{\tau_1}} + A_2 e^{-\frac{t}{\tau_2}} + A_3 e^{-\frac{t}{\tau_3}} + y_0 \quad \text{eq. 2}$$

The mean lifetime value was calculated as:

$$\tau_{mean} = \frac{(A_1 \times \tau_1 + A_2 \times \tau_2 + \dots)}{(A_1 + A_2 + \dots)} \quad \text{eq. 3}$$

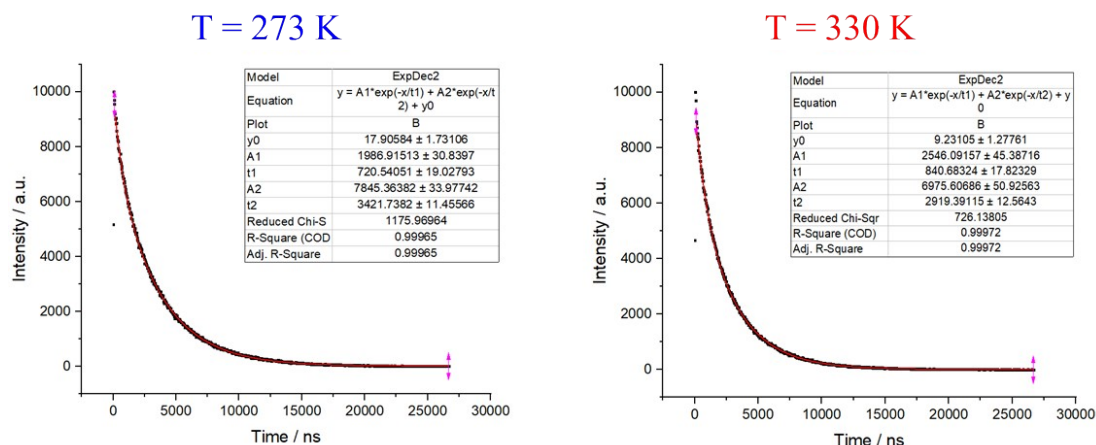


Figure S4.- Excited state decay profiles of **Re** at 273 and 330 K (black dots) and biexponential fits (red).

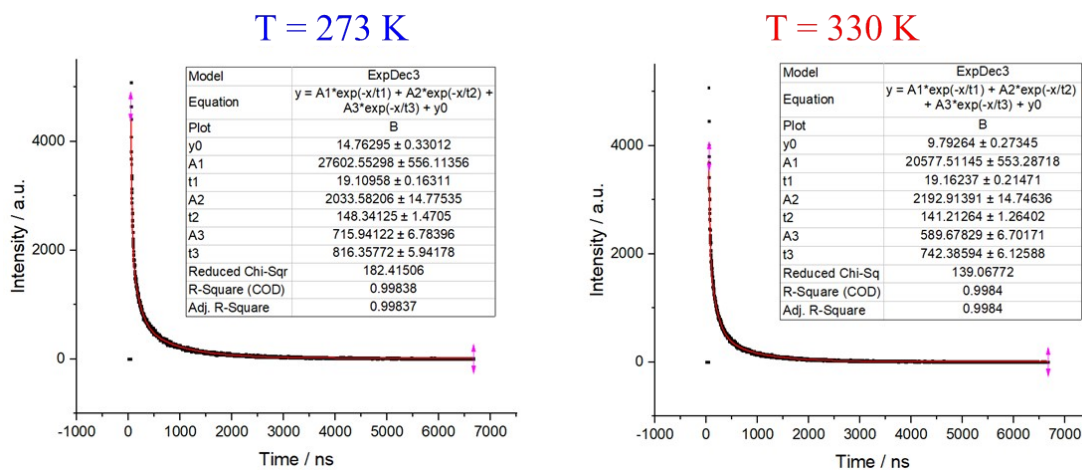


Figure S5.- Excited state decay profiles of **1@SiO₂/Re** at 273 and 330 K (black dots) and biexponential fits (red).

Compounds	τ_1 / ns	τ_2 / ns	τ_3 / ns	<i>A1</i>	<i>A2</i>	<i>A3</i>	$\tau_{\text{mean}}/\text{ns}$
Re (T = 273K)	720	3421	---	1986	7845	---	2875
Re (T = 330 K)	788	2896	---	2502	7083	---	2346
1@SiO₂/Re (T 273K)	17	131	780	28626	1798	620	39
1@SiO₂/Re (T 330K)	15	127	701	37848	2390	701	33

Table S2. Excited-state lifetimes ($\lambda_{\text{ex}} = 395\text{nm}$) of **Re** and **1@SiO₂/Re** in the solid state at T = 273 K and T = 330 K.

6.- Magnetic Properties of sample 1@SiO₂/Re.

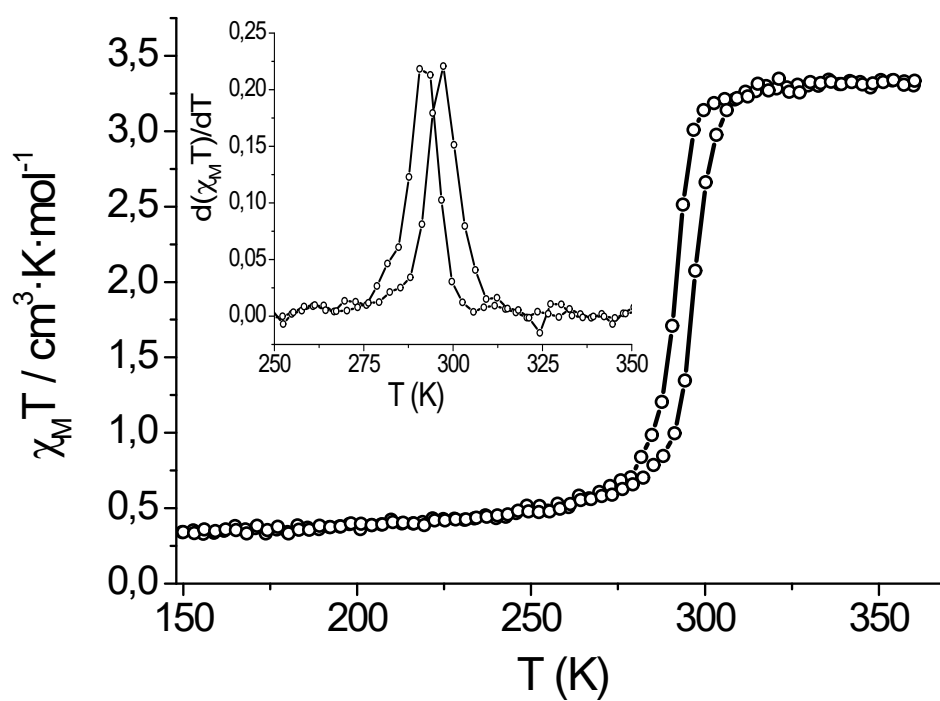


Figure S6. Thermal dependence of the $\chi_M T$ product for sample 1@SiO₂/Re under an applied magnetic field $H_{dc} = 1$ T.

3.- Thermal dependence of the excitation spectrum for sample 1@SiO₂/Re.

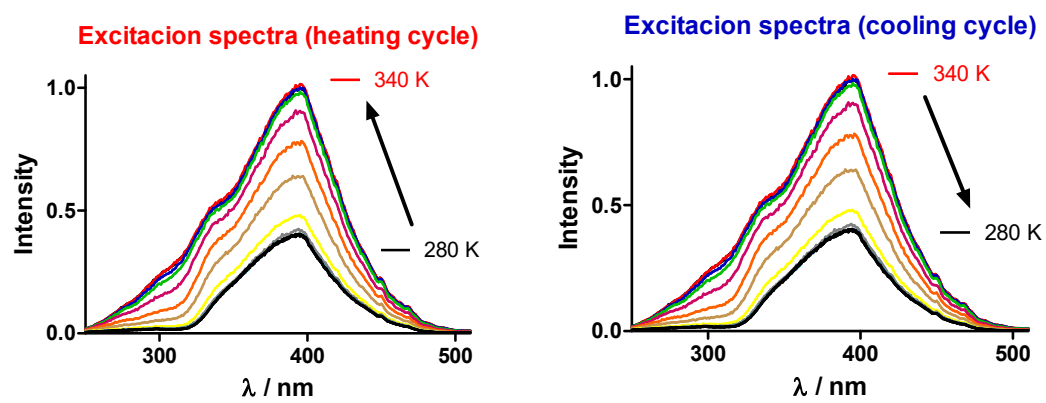


Figure S7.- Variation of the excitation spectra of 1@SiO₂ upon heating (left) and cooling (right) cycles.