

Preserving Spin Transition Properties of Iron-Triazole Coordination Polymers Within Silica-Based Nanocomposites

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Supplementary Information

- 1. DSC of an amorphous gel and crystalline precipitate**
- 2. XRPD of the suspension at different temperature**
- 3. Effect of silica particles addition and surface chemistry**
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1. DSC OF AN AMORPHOUS GEL AND CRYSTALLINE PRECIPITATE

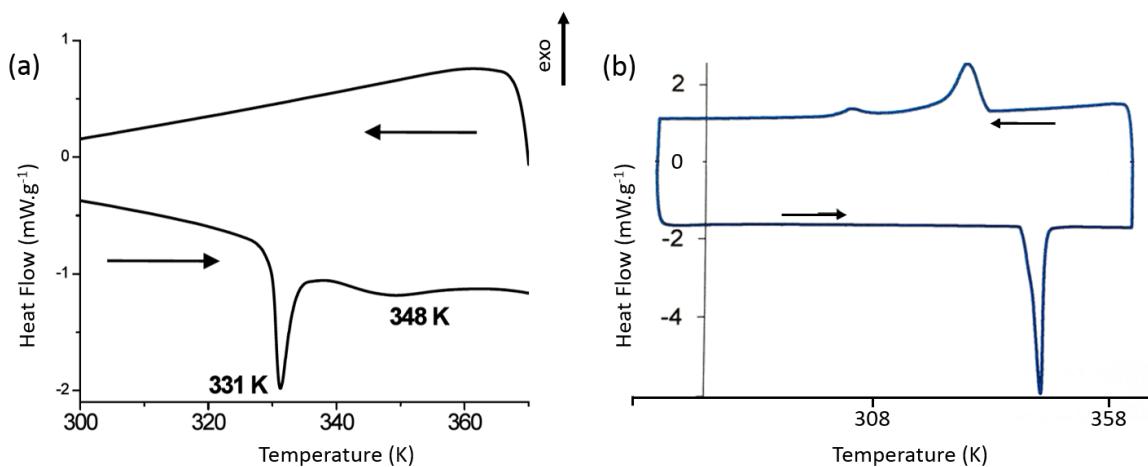


Figure S1. DSC curves performed at scan rate of $5K\cdot min^{-1}$ upon a second cycle (a) for pink $[Fe(HTrz)_3]Br_2$ in glycerol and (b) for pink $[Fe(ATrz)_3](SO_4)$ crystalline precipitate in water.

2. XRPD OF THE SUSPENSION AT DIFFERENT TEMPERATURES

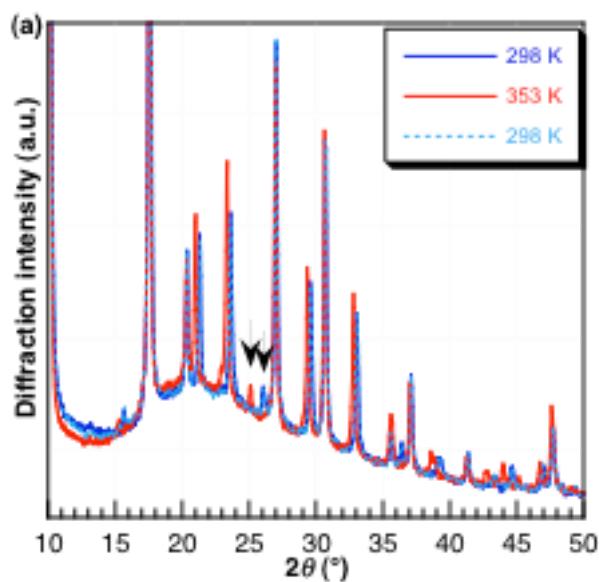


Figure S2. XRPD diffractograms of the 9 days-old $Fe/ATrz/SO_4$ suspension at room temperature (line blue), at $T = 353 \text{ K}$ (red) and at room temperature after the heating/cooling cycle (dashed line blue).

3. EFFECT OF SILICA PARTICLES ADDITION AND SURFACE CHEMISTRY

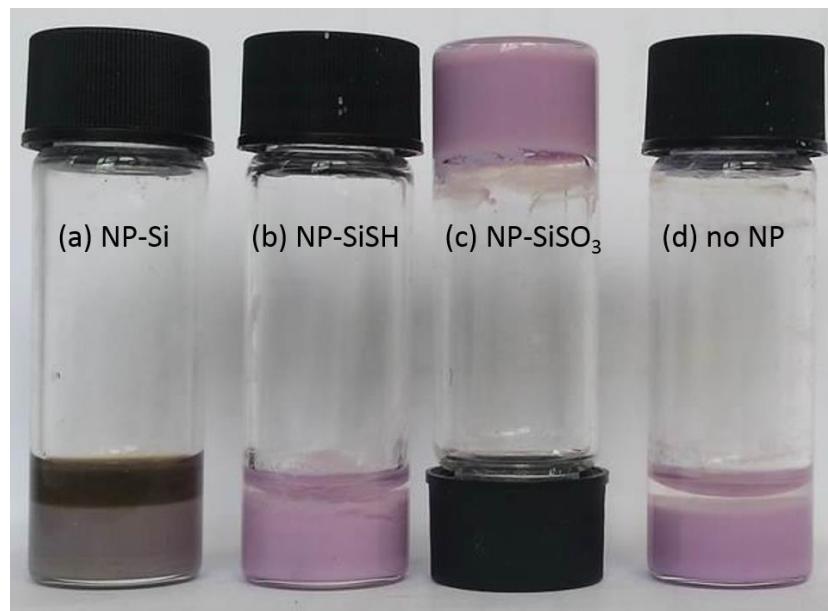


Figure S3. Macroscopic aspect of (a-c) NP-Si@Fe/ATrz/SO₄ composites with different surface chemistry of silica nanoparticles: (a) unmodified silica nanoparticles (NP-Si), (b) thiol-modified silica nanoparticles (NP-SiSH), and (c) sulfonate-modified silica particles (NP-SiSO₃). (d) Macroscopic aspect of Fe/ATrz/SO₄ suspension in absence of nanoparticles.

4. XRPD OF THE COMPOSITE SYSTEM AND OF ITS COMPONENTS

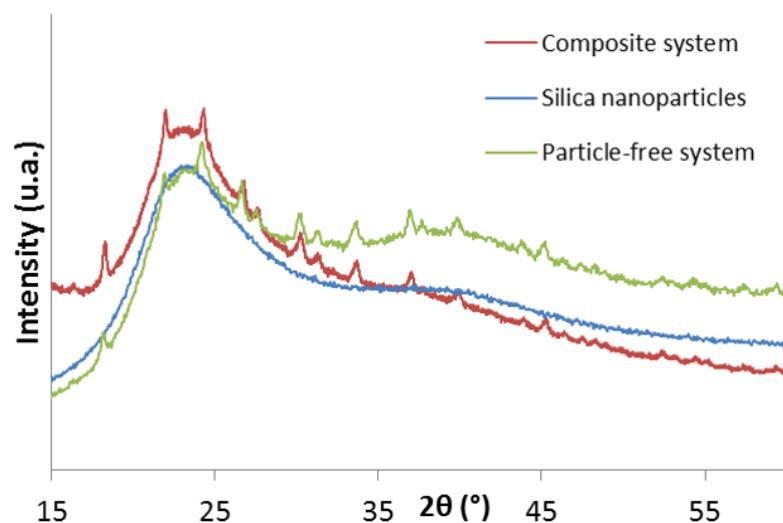


Figure S4. XRPD diffractograms of the 9 days-old NP-SiSO₃@Fe/ATrz/SO₄ composite (red), of the NP-SiSO₃ nanoparticles alone (blue) and of the 9 days-old Fe/ATrz/SO₄ suspension (green).

5. DSC OF Fe/ATrz/SO₄ SUSPENSION AND NP-SiSO₃@Fe/ATrz/SO₄ COMPOSITE

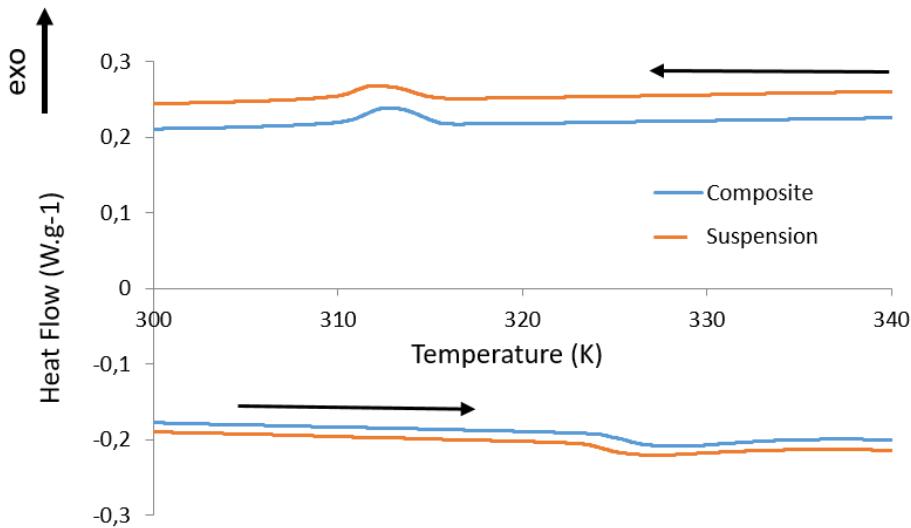


Figure S5. DSC profiles for NP-SiSO₃@Fe/ATrz/SO₄ composite (in blue) and Fe/ATrz/SO₄ suspension (in red) aged for 9 days in a mixture of water/glycerol at scan rate of 5 K.min⁻¹ upon a second thermal cycle.

6. SUMMARY TABLE OF RESULTS FROM DSC AND MAGNETIC MEASUREMENTS FOR THE FOUR SYSTEMS

	Fe/ATrz/SO ₄ Suspension	NP-SiSO ₃ @Fe/ATrz/SO ₄ Composite	DRIED Suspension	DRIED Composite
T ↑ (K) ^a	322	330	343	343
Or T _{max} ↑ (K) ^b	(325)	(328)	(333)	(329)
T ↓ (K) ^a	311	316	329	329
Or T _{max} ↓ (K) ^b	(310)	(315)	(321)	(312)
ΔT (K) ^a	10	14	14	14
Or ΔT (K) ^b	(15)	(13)	(12b)	(17)
ΔH ↑ (kJ.mol ⁻¹)	n.d.	12.5	14.5	14.5
Or ΔH ↑ (kJ.sample g ⁻¹)		(11.1)	(35.3)	(8.7)
ΔH ↓ (kJ.mol ⁻¹)	n.d.	11.9	14.5	14.5
Or ΔH ↑ (kJ.sample g ⁻¹)		(10.6)	(36.0)	(7.9)

Table S1: Transition temperatures on warming and cooling from (a) magnetic and (b) DSC measurements, and thermodynamic parameters for Fe/ATrz/SO₄ suspension, NP-SiSO₃@Fe/ATrz/SO₄ composite and the dried samples (n.d.: not determined).

7. EFFECT OF DRYING AND RESOLVATION OF THE Fe/ATrz/SO₄ SUSPENSION

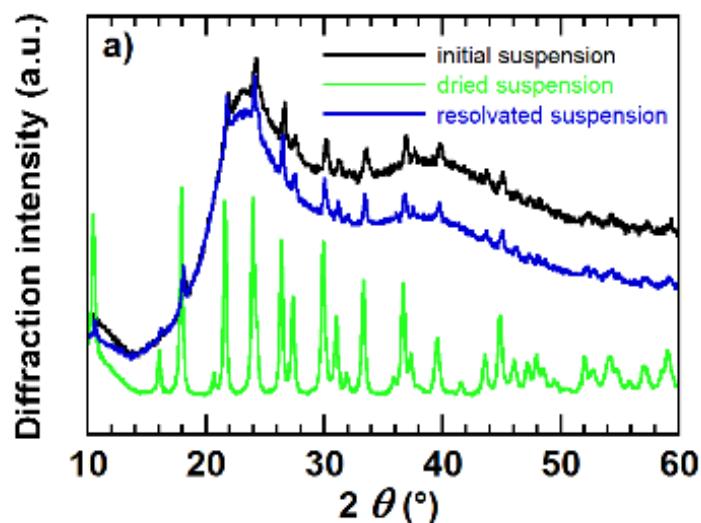


Figure S6. XRPD diffractograms of the initial Fe/ATrz/SO₄ suspension (in black), the dried suspension powder (in green) and the resolvated suspension (in blue).

8. DSC PROFILES OF THE DRIED AND RESOLVATED SAMPLES

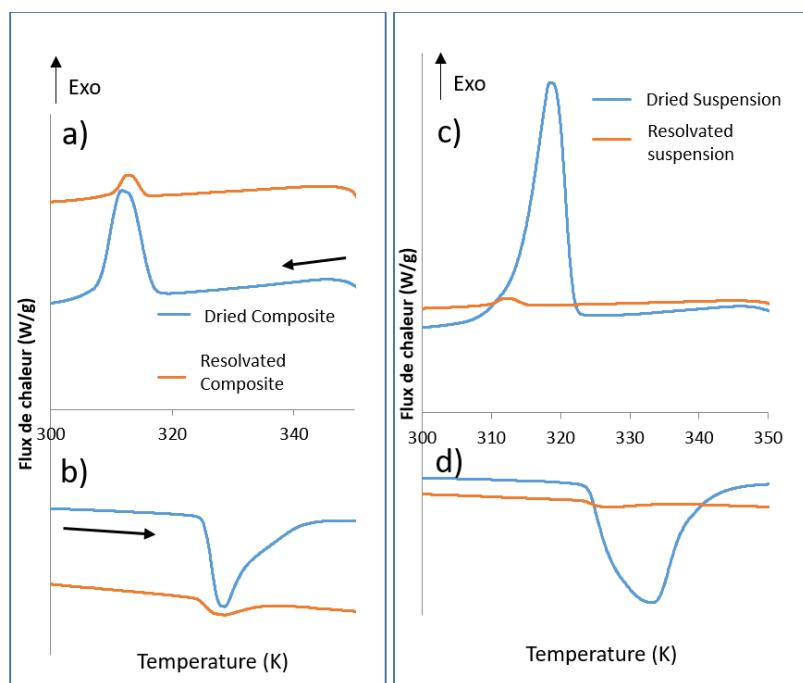


Figure S7. DSC Profiles for the dried (in blue) and resolvated (in red) samples of NP-SiSO₃@Fe/ATrzSO₄ composite or Fe/ATrz/SO₄ suspension studied on warming (b and d) and cooling (a and c) at variable temperatures with a scan rate of 5K.min⁻¹ upon a second thermal cycle.