Electronic Supplementary Material (ESI) for CrystEngComm.

Effect of precursor concentration on size evolution of iron oxide nanoparticles

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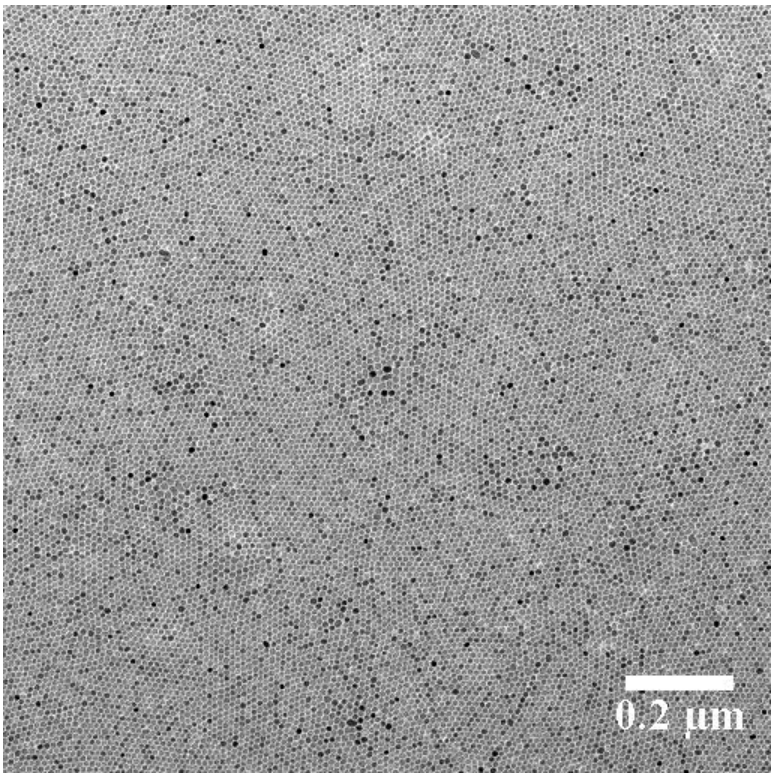

Figure S1. Large scale bar image of standard sample.

Information on XRD:

Calculation the crystalline size via Scherrer's formula:

The crystallite size of Nanoparticles for the most intense, (311) plane was determined from the X-ray data using Debye–Scherrer formula:[1]

(1) $D = K\lambda/\beta Cos\Theta$

where λ is the wavelength of X-ray (λ=1.5406 Å); β the full width at half maximum (obtained from fitting the 311 peak); Θ is the Bragg's diffraction angle (around 35°-obtained from fitting the 311 peak) and K is the shape factor which is normally taken as 0.9-1 for ferrites.

The interplaner distances d_{hkl} (A˚) were calculated using Bragg's law[2] and then the lattice constant of the samples was calculated using the relation:

(2) $n\lambda = 2d\sin\theta$

(3) $a = d_{hkl}\sqrt{h^2+k^2+l^2}$

where a is lattice constant; (hkl) is the indexing plane of atoms which can be obtained from X-ray diffraction data.[1, 3]

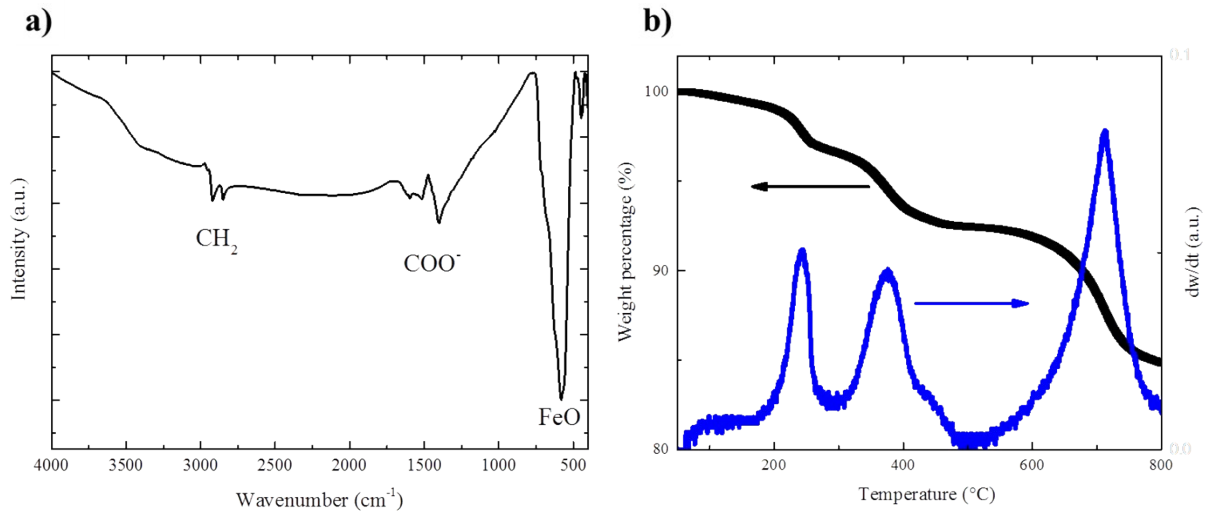

Figure S2. (a) IR spectrum of standard samples between 4000 to 400 cm-1, (b) TGA and DTG graph of standard samples between 25 °C to 800 °C.

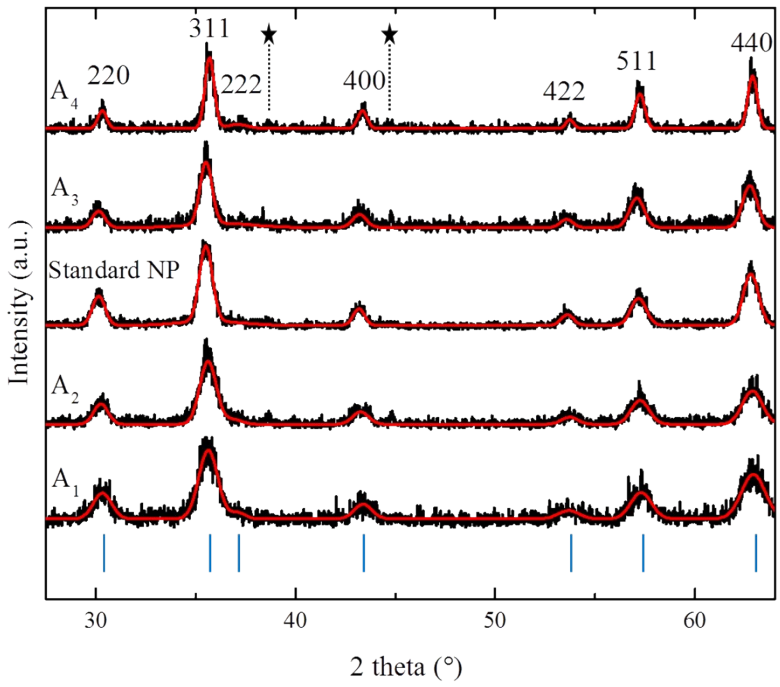

Figure S3. XRD patterns of five batches of Nanoparticles (black data) and their corresponding modelisations (red data). Positions of the Bragg reflections are represented by vertical blue bars. Holder reflections are indicated by stars.

Calculation the graft density:

The amount of grafting was calculated from the TGA and DTA data, according to the following equations:

(4) Number of surfactants (molecules) $$N_s = \frac{m_1 - m_3}{M} \times N_A$$

(5) Number of Nanoparticles $$N_P = \frac{m_3}{\rho \times V}$$

(6) Graft density (molecules/nm^2) $$G.D. = \frac{N_s}{N_P \times A}$$

where m_1 and m_3 are the amount of mass in the first and third DTA peaks, ρ is the density of Nanoparticles (~ 5.18 g/cm^3), M is the molecular weight of capped surfactant (282.46 g/mol), V is the volume of each individual NP and A is the average are of single NP.

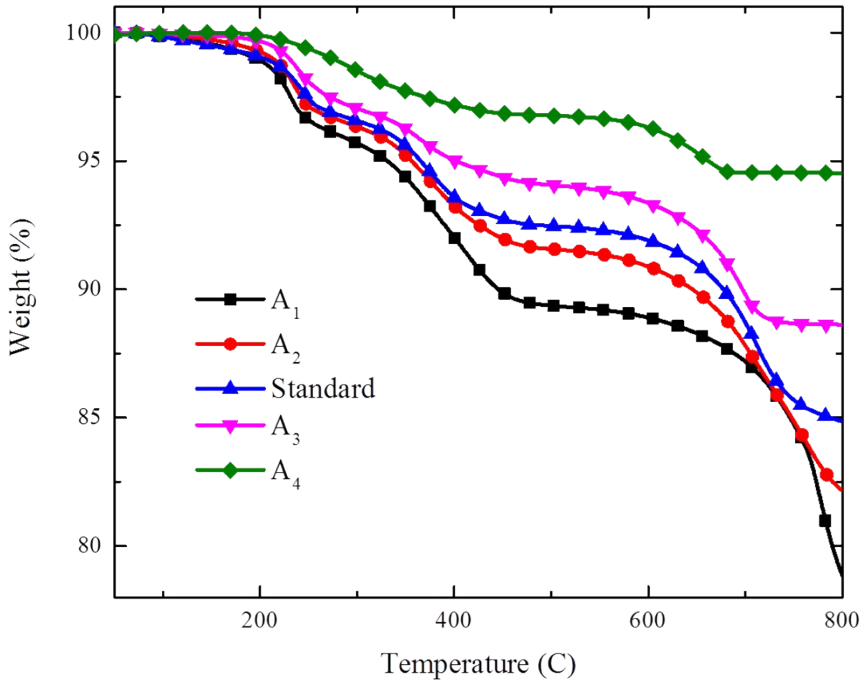

Figure S4. TGA graphs of the samples B_1-B_4 from 30-800 °C.

Table 1. Weight loss percentage and graft density of the samples B_1-B_4 and standard sample from TGA.

Sample name	Volume of solvent (ml)	Size (nm)	Weight loss (%)	Graft density (molecules/nm^2)
A_1	28	9.1 ± 0.71	18.1	3.6 ± 0.1
A_2	24	10.5 ± 1.08	15.7	3.6 ± 0.2

Standard	20	13.0 ± 1.1	12.2	3.3 ± 0.2
A_3	16	15.1 ±1.4	10.7	3.3 ± 0.2
A_4	12	24.1 ± 5.7	5.5	2.7 ± 0.3

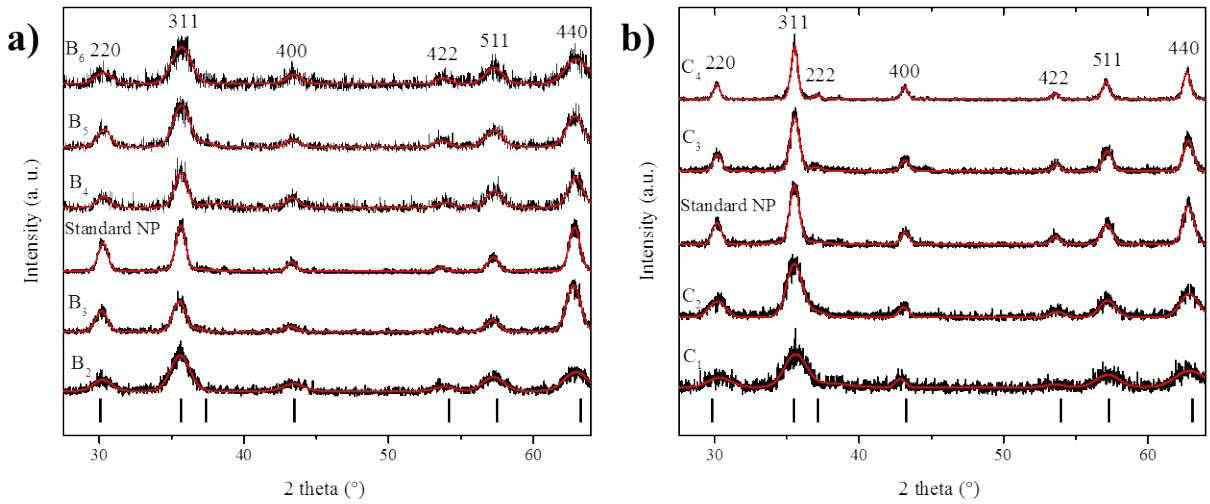

Figure S5. XRD patterns of samples series B (a) and C (b) (black data) and their corresponding modelisations (red data). Positions of the Bragg reflections are represented by vertical black bars.

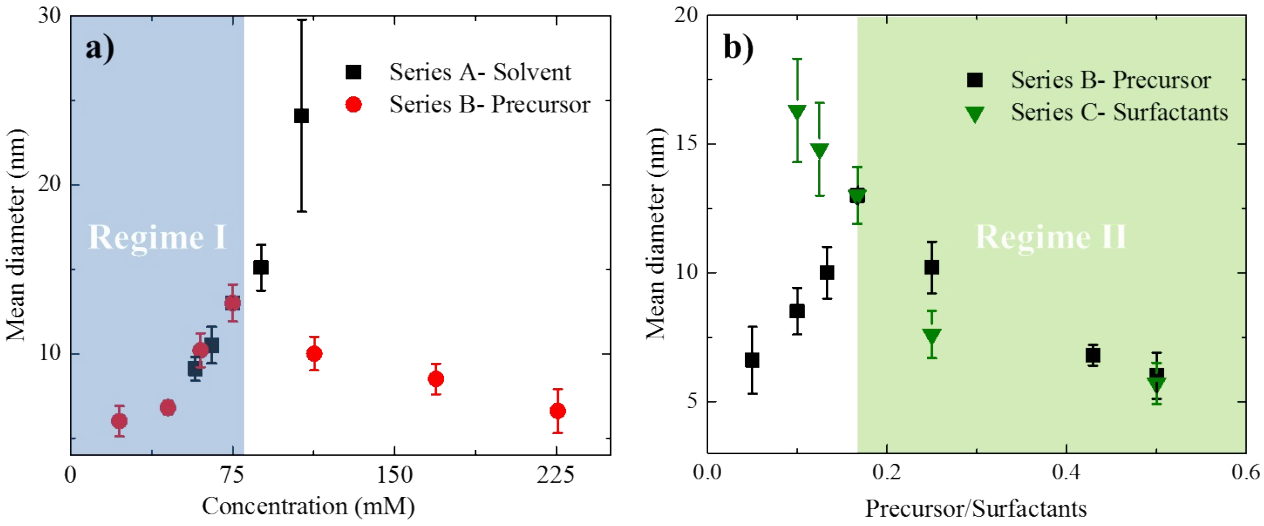

Figure S6. The evolution of mean diameter as function of (a) precursor concentration and (b) precursor to surfactants ratio.

References

1. G. Arrhenius, *J. Chem. Educ*, 1955, **32**, 228-229.
2. K. Venkatesan, D. R. Babu, M. P. K. Bai, R. Supriya, R. Vidya, S. Madeswaran, P. Anandan, M. Arivanandhan and Y. Hayakawa, *Int. J. Nanomed.*, 2015, **10**, 189-198.
3. Y. Eom, M. Abbas, H. Noh and C. Kim, *RSC Adv.*, 2016, **6**, 15861-15867.