

Modulation of hyperthermic and relaxometric responses of magnetic iron oxide nanoparticles through ligand exchange provides design criteria for dual-functionality

Esther Rani Aluri,[†] Sameer D. Shingte,^{1†} Eoin P. McKiernan,¹ Steven Ferguson,² Dermot F. Brougham^{1*}

1. School of Chemistry, University College Dublin, Belfield, Dublin 4, Ireland.

2. School of Chemical and Bioprocess Engineering, University College Dublin, Belfield, Dublin 4, Ireland.

Supplementary information

Table S1: SAR, hydrodynamic size, and particle sizes of OA/OAm-MNP suspensions (toluene) synthesised by modifying in the reaction steps, precursor to surfactant ratio, and varying the passage of gas. For the above reaction procedures, precursor and solvent were used from the same source.

A. Modifications in reagents/gas	SAR (W g ⁻¹)	DLS		TEM	
		<i>d_{hyd}</i> (nm)	<i>PDI</i>	<i>d_{core}</i> (nm)	St Dev (%)
Reaction in Ar gas	76	20	0.11	-	-
Dry octyl ether (Dried on 3 Å molecular sieves)	731	26	0.13	-	-
Octyl ether added from glove box	398	21	0.09	-	-
B. Modifications in reaction steps					
Direct reflux 1h-N ₂ atm (No hold at 200 °C) Same as Cheon	318	23	0.29	16.3	4.8
Direct reflux 1h- atm (No hold at 200 °C)	201	20	0.19	17.3	3.1
Reflux 2h- N ₂ atm (Hold at 200 °C; 1 h)	175	18	0.14	15.9	2.9
Reflux 1h- N ₂ atm (Degas 110 °C- 30 min Hold at 200 °C- 1 h)	60	21	0.13	-	-
C. Modifications in precursor to surfactant ratio					
Fe(acac) ₃ : Surfactants 1:4	43	28	0.13	-	-
Fe(acac) ₃ : Surfactants 1:5	63	21	0.08	-	-

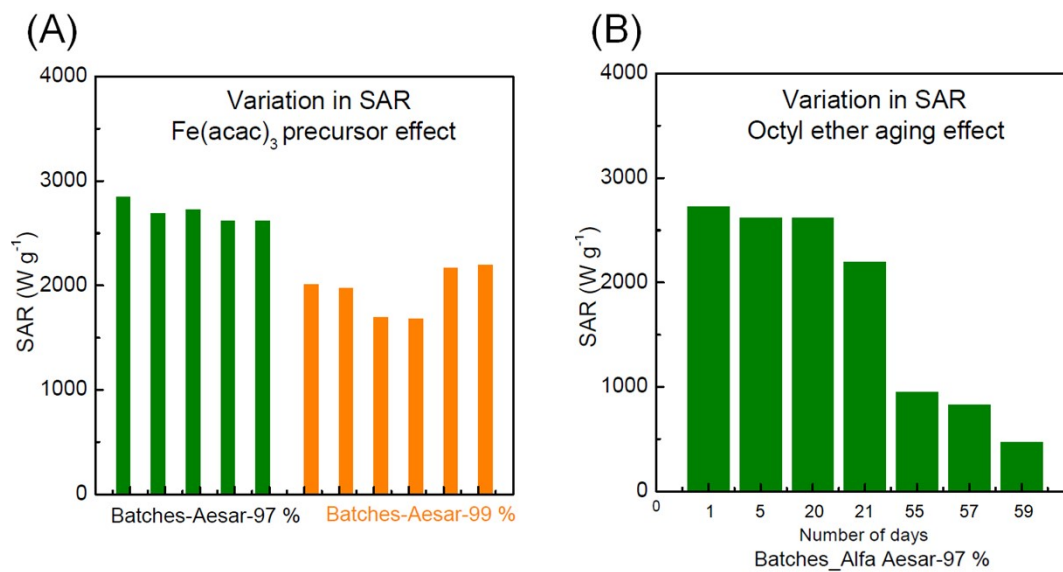


Figure S1: Reproducibility of the optimised OA/OAm-MNP synthesis protocol. (A) Variation in SAR values obtained for OA/OAm-MNP suspensions prepared using iron (III) precursors from different sources. (B) SAR variation with ageing (time after opening the bottle) of the octyl ether reaction solvent.

Table S2: SAR values (at 535 kHz, 16 kA m⁻¹) of OA/OAm-MNP toluene suspensions, colloidal characterisation in toluene, and TEM characterisation of multiple batches prepared using different precursor sources.

Precursor source	SAR (W g ⁻¹)	DLS		TEM	
		<i>d</i> _{hyd} (nm)	<i>PDI</i>	<i>d</i> _{TEM} (nm)	Std.dev. (%)
Fe(acac)₃, Alfa Aesar, 97%	2844	28	0.15	16.1±0.6	3.7
	2692	24	0.19	-	-
	2726	25	0.18	15.2±0.7	4.7
	2620	28	0.28	-	-
	2620	23	0.18	16.2±1.0	5.9
Fe(acac)₃, Alfa Aesar, 99%	2013	19	0.09	-	-
	1977	21	0.14	-	-
	1698	26	0.09	15.5±2.0	12.9
	1681	22	0.07	-	-
	2164	23	0.13	16.0±0.6	3.7
	2195	24	0.11	-	-

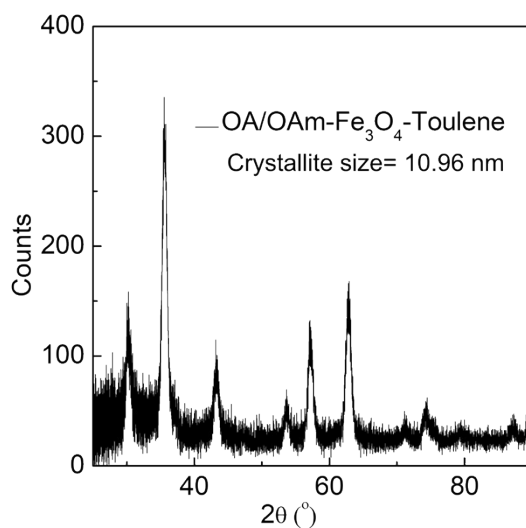


Figure S2: XRD patterns of OA/OAm-MNPs with a crystallite size of 11.0 nm

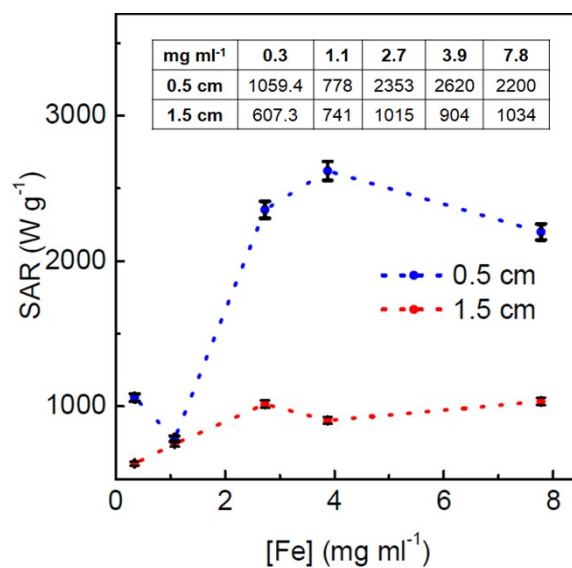


Figure S3: SAR as a function of Fe concentration, measured with the thermal probe placed at 0.5 and 1.5 cm from the bottom for the same OA/OAm-MNP suspension.