

## SUPPLEMENTARY INFORMATION

# Susceptibility losses in heating of magnetic core/shell nanoparticles for hyperthermia: A Monte Carlo study of Shape and Size effects

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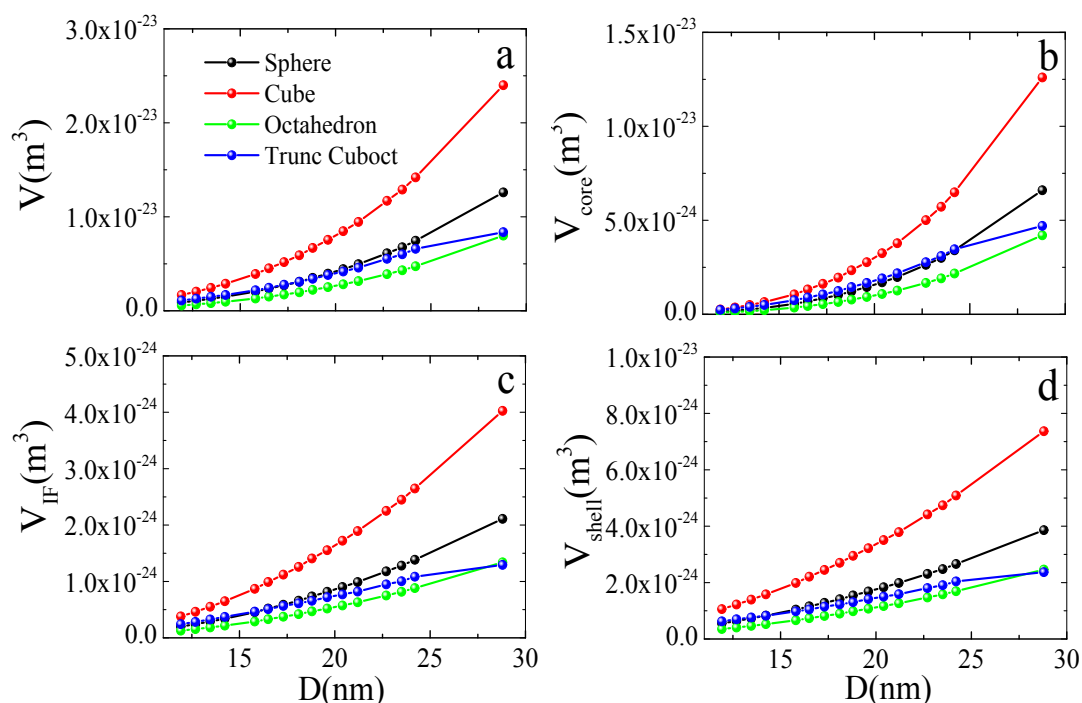
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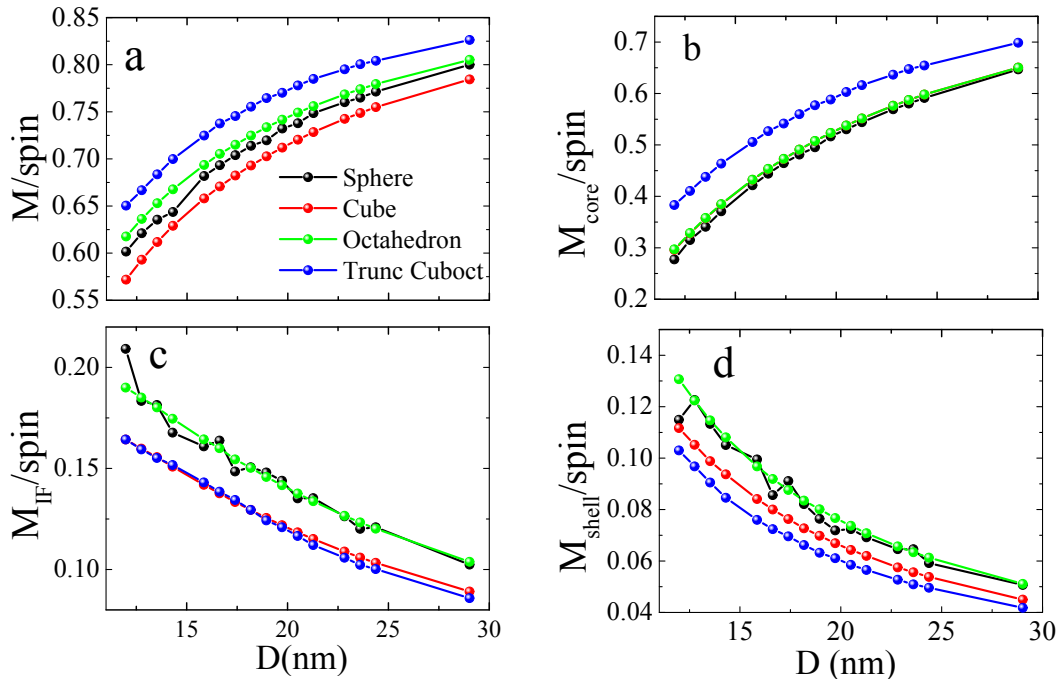
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### Calculations of the total volume and the volume of the core, interface, shell of FM/FiM and FiM nanoparticles as a function of the nanoparticle size, for the four shapes.

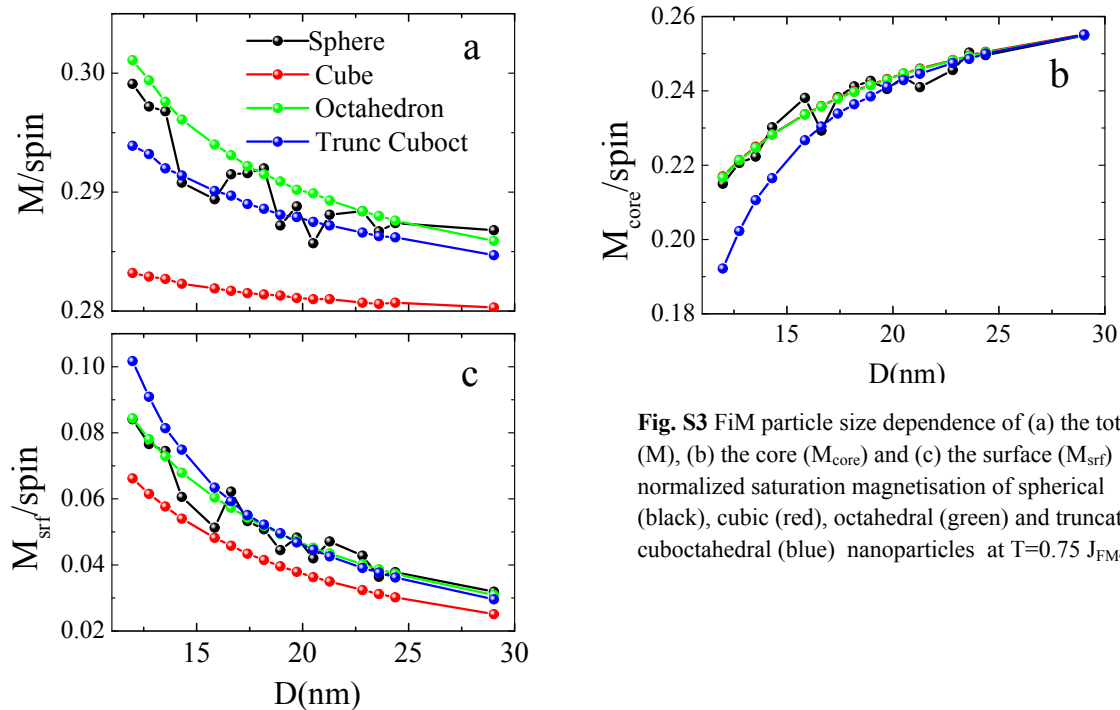


**Fig. S1** (a) The total magnetic volume ( $V$ ), (b) the core volume ( $V_{\text{core}}$ ), (c) the interface volume ( $V_{\text{IF}}$ ) and (d) the shell volume ( $V_{\text{shell}}$ ) as a function of nanoparticle size ( $D$ ) of spherical (black), cubic (red), octahedral (green) and truncated cuboctahedral (blue) FM/FiM nanoparticles with shell thickness 2.5 nm.

## Monte Carlo simulations of the magnetisation for FM/FiM and FiM nanoparticles of different sizes and shapes

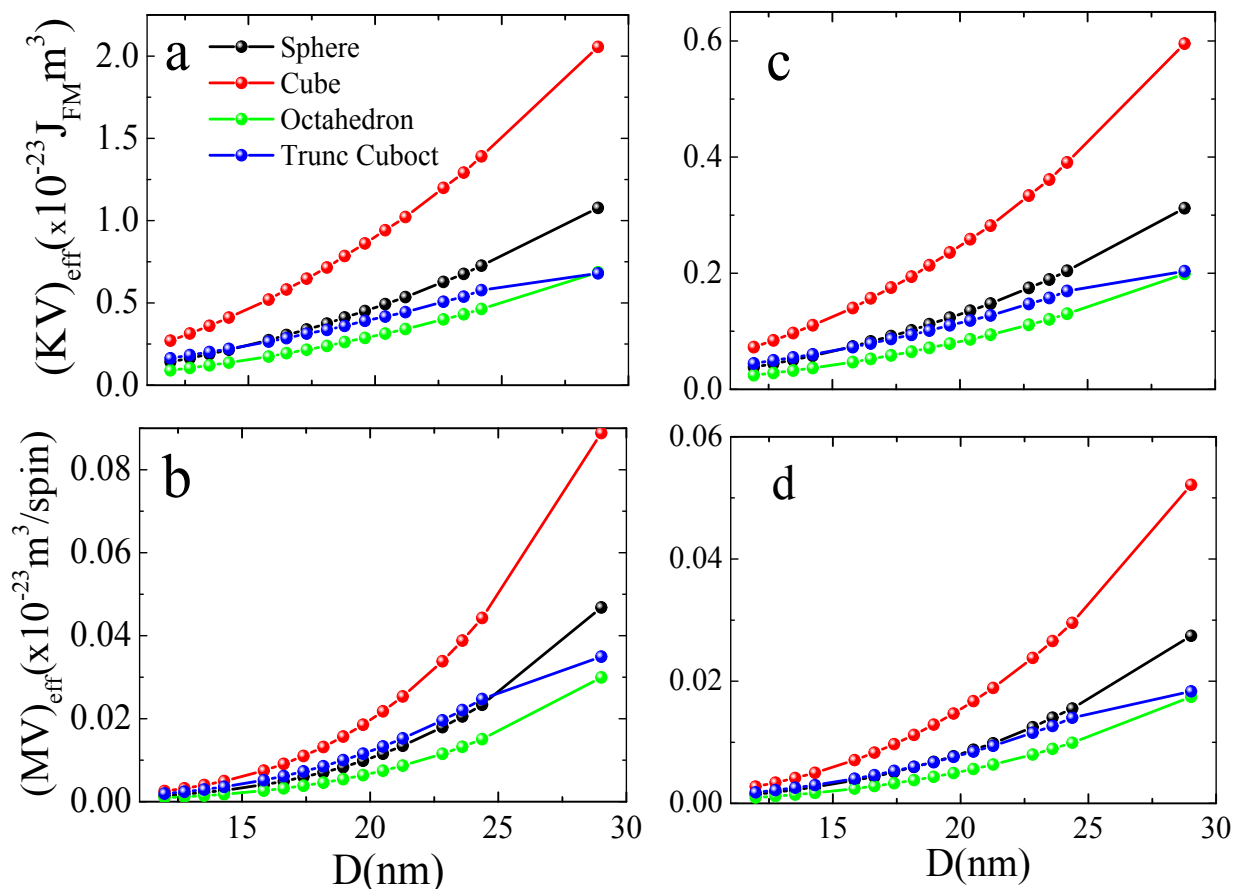


**Fig. S2** FM/FiM nanoparticle size dependence of (a) the total ( $M$ ), (b) the core ( $M_{\text{core}}$ ), (c) interface ( $M_{\text{IF}}$ ) and (d) shell ( $M_{\text{shell}}$ ) normalized saturation magnetisation of spherical (black), cubic (red), octahedral (green) and truncated cuboctahedral (blue) with FiM shell thickness 2.5 nm at  $T=0.75 J_{\text{FM}}/k_{\text{B}}$ . The details of the structure of each region affect the calculated saturation magnetisation, so the reduced symmetry mainly in the interface and the shell of the spherical shape causes the observed fluctuations of the magnetic component in these regions and consequently to the total magnetisation.



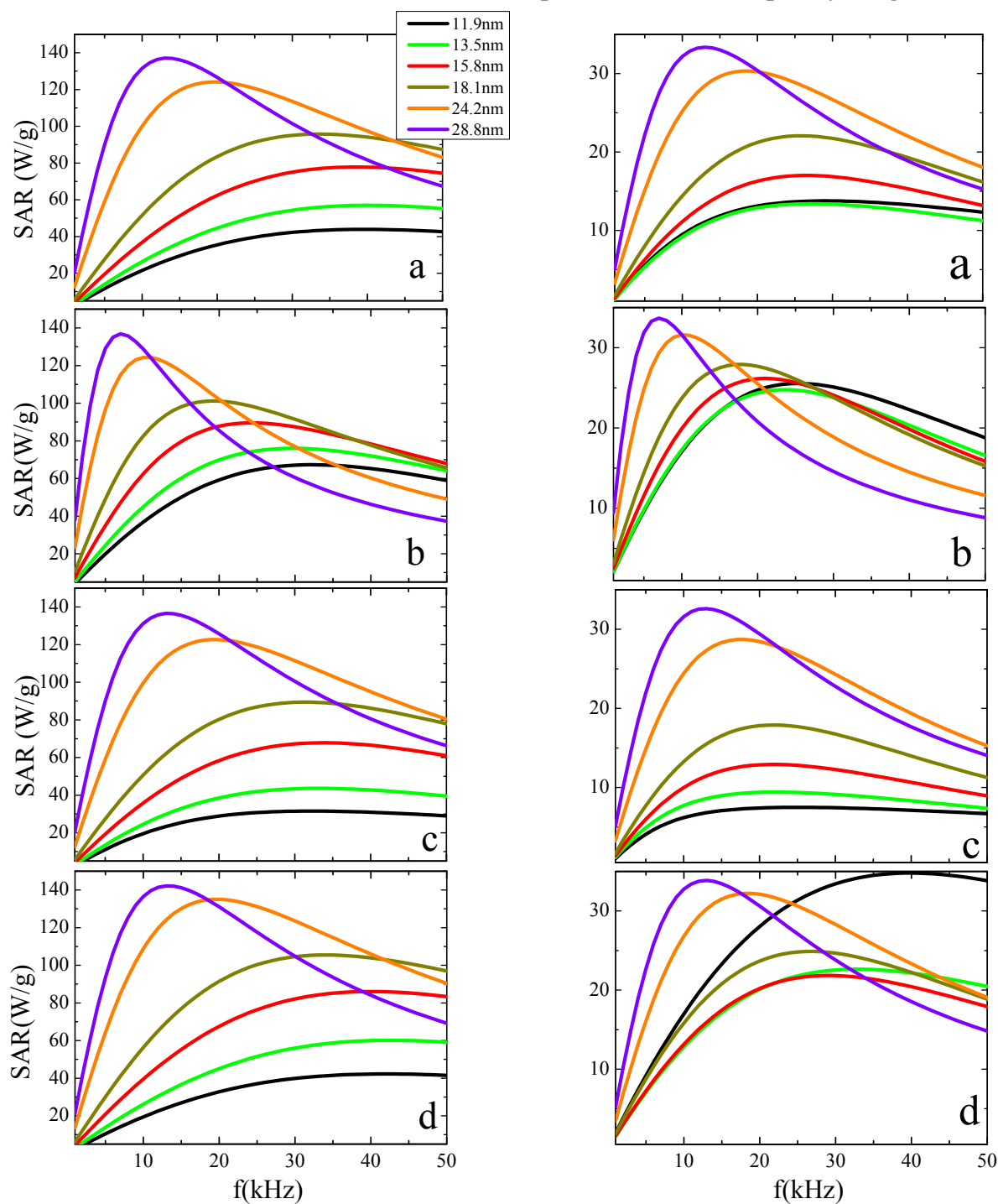
**Fig. S3** FiM particle size dependence of (a) the total ( $M$ ), (b) the core ( $M_{\text{core}}$ ) and (c) the surface ( $M_{\text{srf}}$ ) normalized saturation magnetisation of spherical (black), cubic (red), octahedral (green) and truncated cuboctahedral (blue) nanoparticles at  $T=0.75 J_{\text{FM}}/k_{\text{B}}$

### Calculation of the effective volume anisotropy $(KV)_{\text{eff}}$ and volume magnetisation $(MV)_{\text{eff}}$ for FM/FiM and FiM nanoparticles



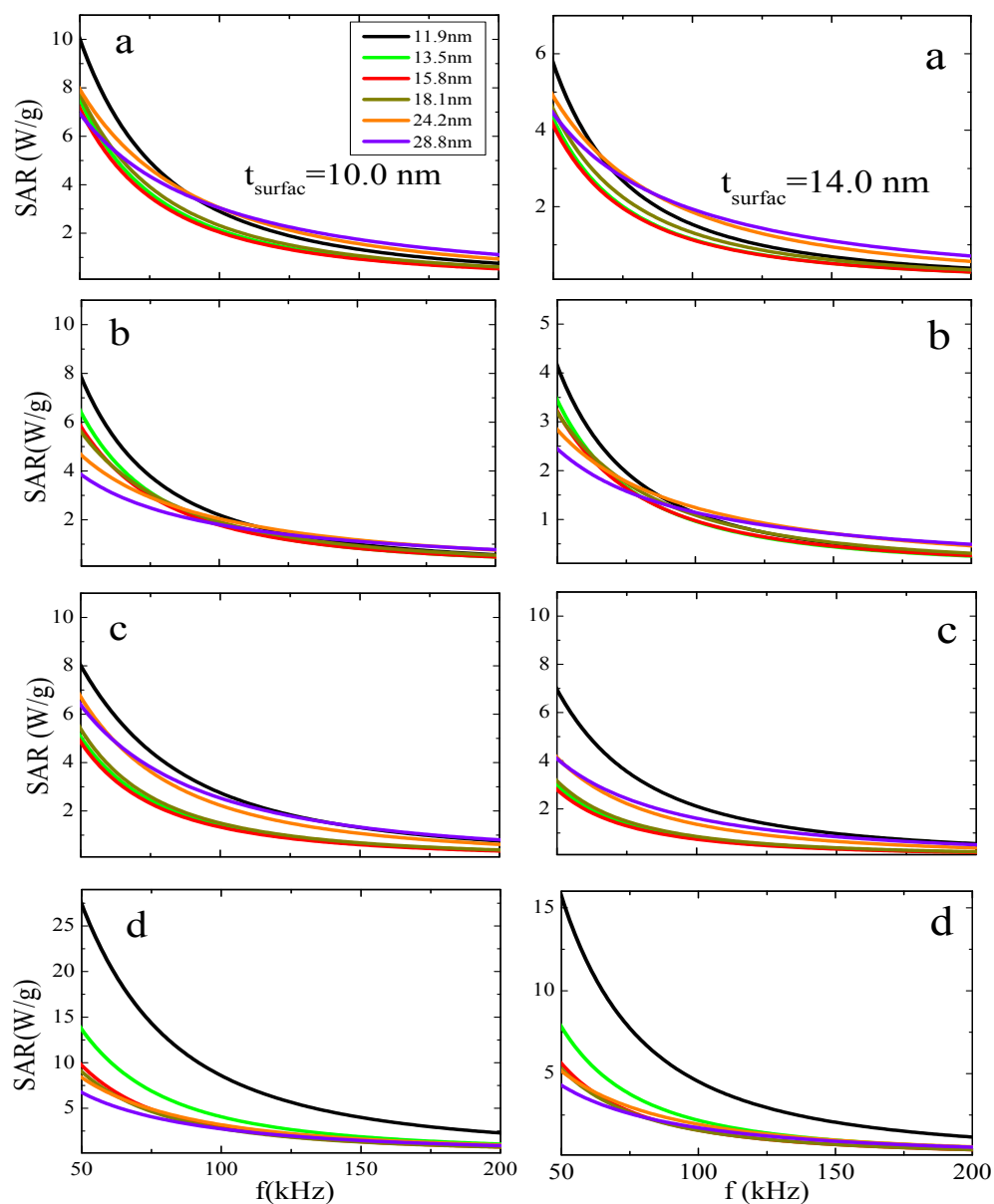
**Fig. S4** (a) The effective volume anisotropy  $(KV)_{\text{eff}}$  and the effective volume magnetisation  $(MV)_{\text{eff}}$  as a function of nanoparticle size ( $D$ ) of spherical (black), cubic (red), octahedral (green) and truncated cuboctahedral (blue) FM/FiM (a,b) and FiM (c,d) nanoparticles.

### Calculations of the SAR for FM/FiM and FiM nanoparticles for the frequency range of 0 - 50 kHz



**Fig. S5** SAR due to susceptibility losses of FM/FiM (left side figures) and FiM (right side figures) spherical (a), cubic (b), octahedral (c) and truncated cuboctahedral (d) nanoparticles with 4 nm surfactant thickness, as a function of the AC magnetic field frequency for different sizes, ( $H_0 \times f = 4.85 \times 10^8 \text{ Am}^{-1}\text{s}^{-1}$ ).

### Calculations of the SAR dependence on surfactant thickness for FiM nanoparticles



**Fig. S6** SAR due to susceptibility losses of spherical (a) cube (b) octahedral (c) and truncated cuboctahedral (d) FiM nanoparticle with surfactant thickness  $t_{\text{surf}} = 10$  nm (left side figures), and  $t_{\text{surf}} = 14$  nm (right side figures) as a function of the AC magnetic field frequency for different sizes following  $H_0 \times f = 4.85 \times 10^8 \text{ Am}^{-1}\text{s}^{-1}$  (safe for application in humans).