Magnetic properties modeling of functionalized magnetite nanoparticles

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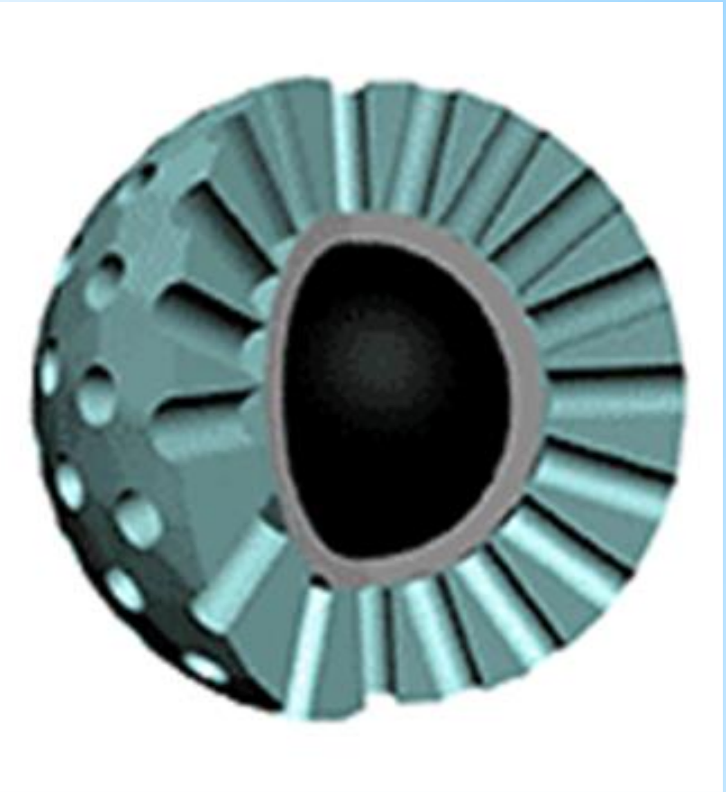
Motivation

Magnetite (Fe_3O_4) nanoparticles

- superparamagnetism
- stability
- biocompatibility
- easy synthesis & modification
- low-cost production



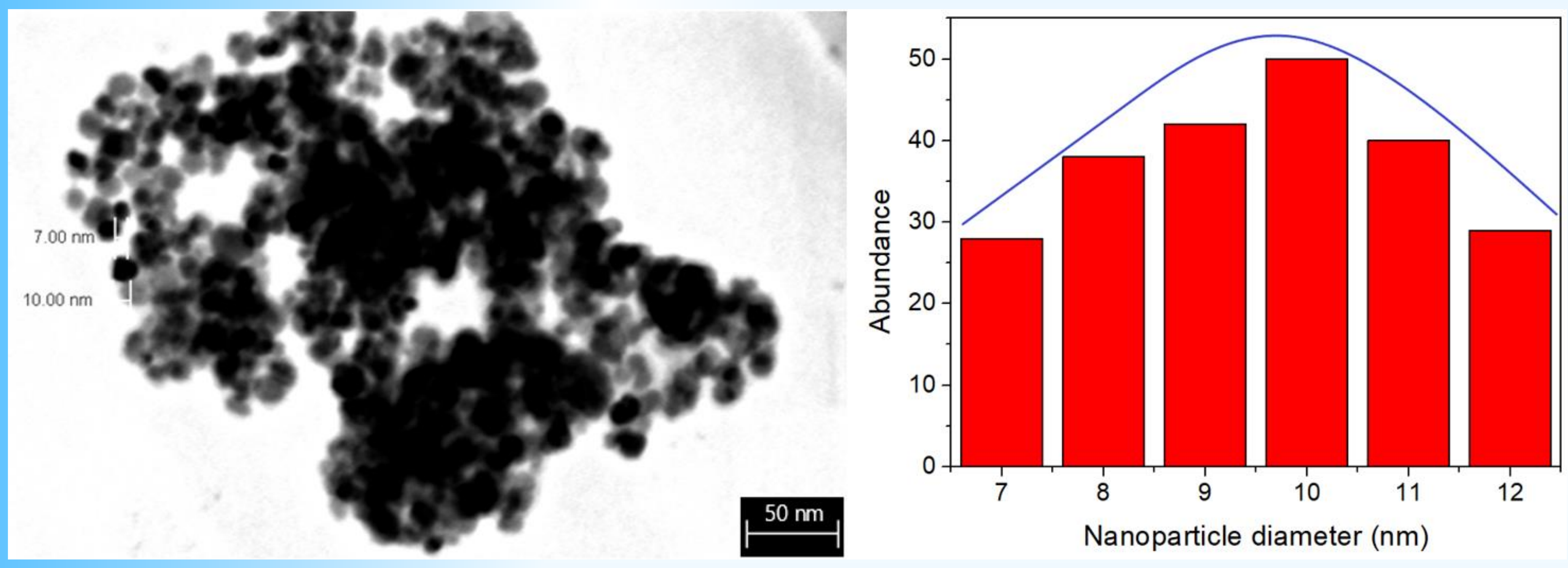
- therapeutic agents in tumor treatment and drug delivery
- MRI contrast media (SPION)
- theranostics

Objectives of the work

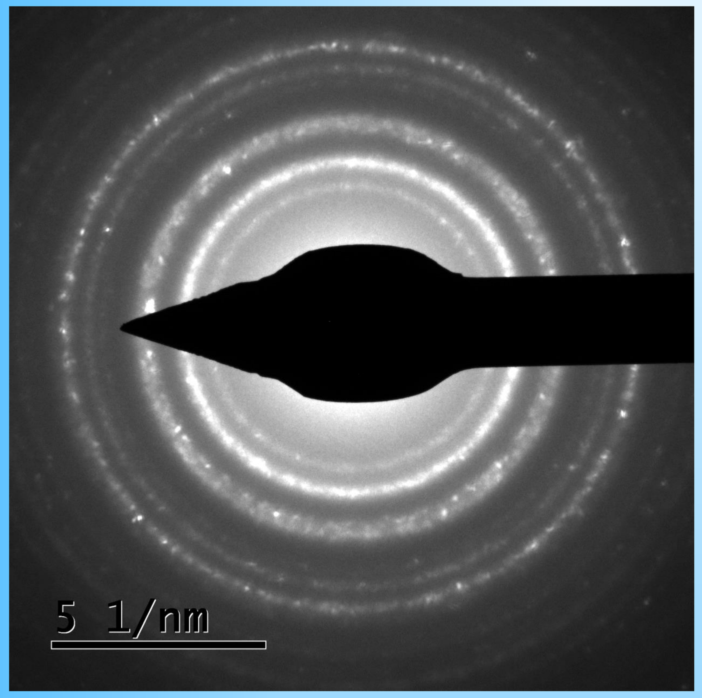
- Determine magnetic size of the particles
- Reveale the possible presence of inter-particle interactions
- Apply and modify an appropriate model to fit the data

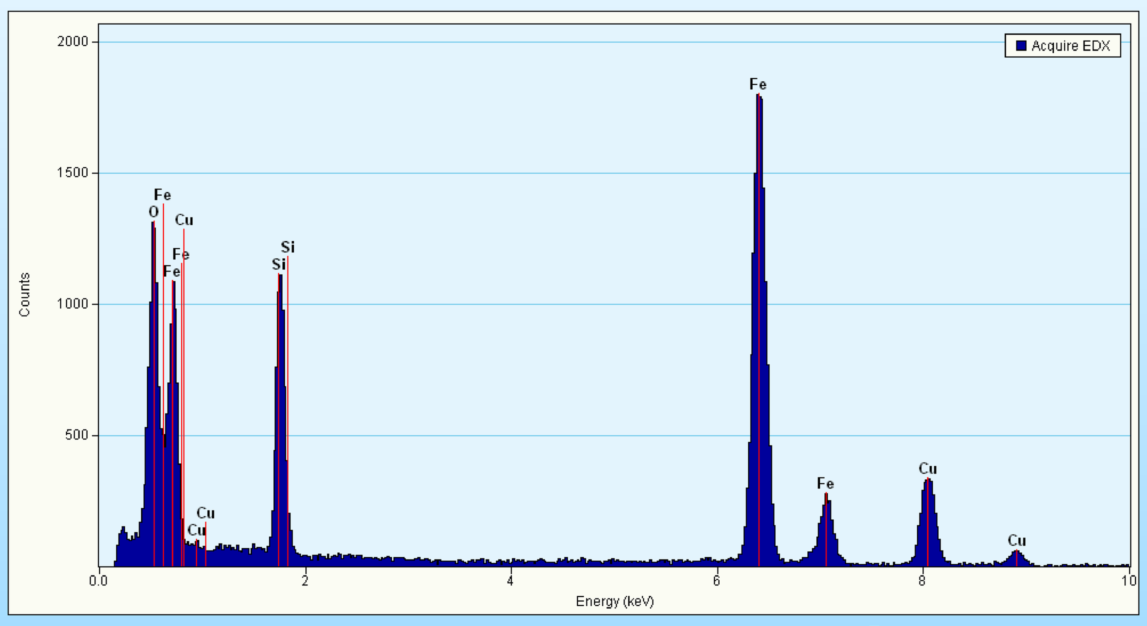
Material

- Fe_3O_4 NPs coated by amorphous silica (**SiO_2**)
- prepared by co-precipitation method

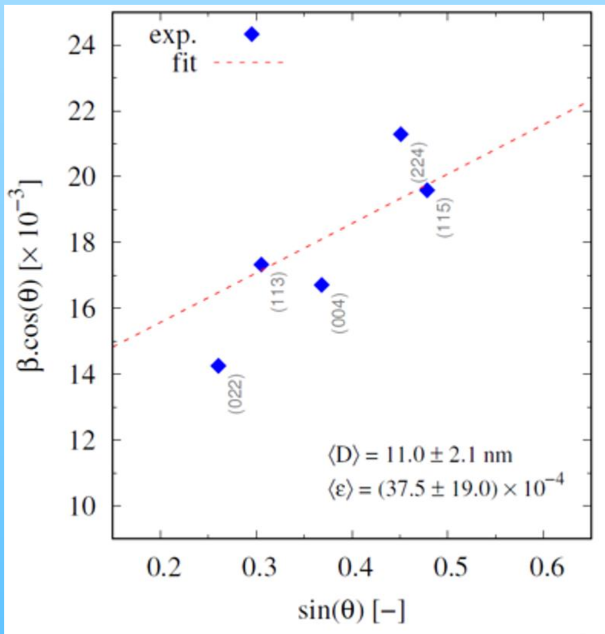


- Transmission electron micrograph of the examined system & corresponding particle size distribution





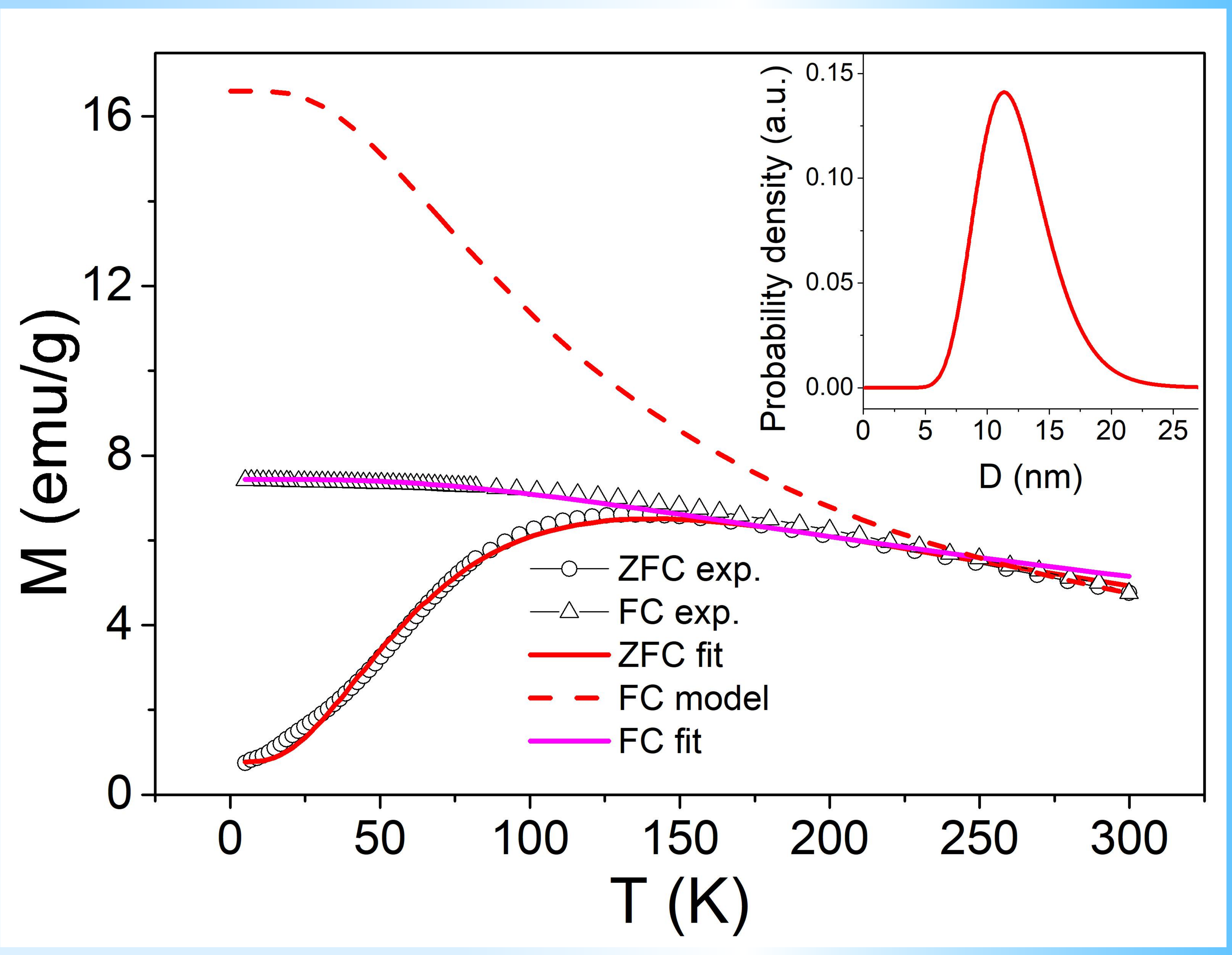
- Energy Dispersive X-Ray Analysis



- X-ray diffraction pattern
- Discrete circles - Fe_3O_4
- Diffuse halo – amorphous SiO_2
- Williams-Hall method: D ~ 11 nm

Magnetic properties modeling

ZFC-FC magnetization data, models & fits



Proposed model description

Assumptions

- superparamagnetic system
- no interactions
- linear field response
- uniaxial particle anisotropy
- lognormal particle volume distribution

$$\rho(V) = \frac{1}{V\sigma\sqrt{2\pi}} exp\left\{-\frac{1}{2}\left[\frac{\ln(V/V_m)}{\sigma}\right]^2\right\} \qquad V_{\lim}(T) = \frac{\gamma k_B T}{K_{\text{eff}}}$$

$$M_{ZFC} = \frac{\mu_0 H \mathcal{M}_S^2}{3k_B T}\int_{V_{\lim}}^{0} V^2\rho(V)\,\mathrm{d}V + \frac{\mu_0 H \mathcal{M}_S^2}{3K_{\text{eff}}}\int_{V_{\lim}}^{\infty} V\rho(V)\,\mathrm{d}V$$

$$M_{FC} = \frac{\mu_0 H \mathcal{M}_S^2}{3k_B T}\int_{0}^{V_{\lim}} V^2\rho(V)\,\mathrm{d}V + \frac{\mu_0 H \mathcal{M}_S^2}{3K_{\text{eff}}}\int_{V_{\lim}}^{\infty} \alpha V\rho(V)\,\mathrm{d}V$$

Results

M_s(core) = 70 emu/g (fixed);

1.) ZFC fit: D_m=13 nm; σ = 0.21; $K_{eff} = 1.8\times10^4$ J/m³

2.) FC model –> discrepancy with experiment

3.) FC fit: D_m=13 nm; σ = 0.25; $K_{eff} = 4.5\times10^4$ J/m³

Conclusions

fits of the model to the exp. data:

- Particle size distribution accords with TEM, XRD
- Discrepancies in the K_{eff} (ref. $K_{eff} \in (1,2)\times10^4$ J/m³)
- Strong inter-particle interactions are reflected in the significant increase of K_{eff}

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