Supplementary Information

Evaluation of Hyperthermia of Magnetic Nanoparticles by Dehydrating DNA

Lina Yu[1, 2], Jinming Liu[2], Kai Wu[2], Todd Klein[2], Yong Jiang[1] and Jian-Ping Wang[2]**

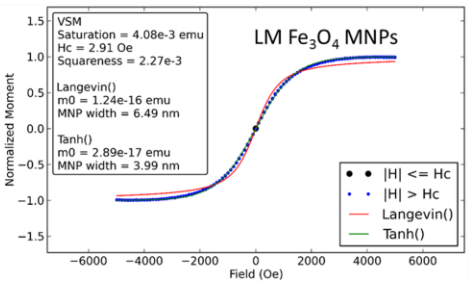
[1]State Key Laboratory for Advanced Metals and Materials, School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing, 100083, China.

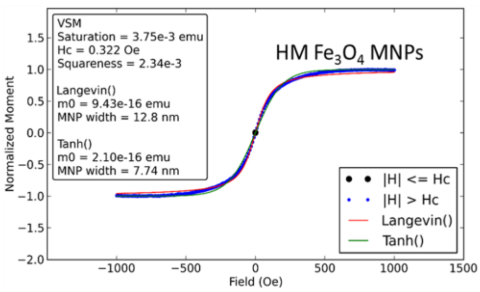
[2]Department of Electrical and Computer Engineering, University of Minnesota, Minneapolis, MN. 55455, USA.

*E-mail: jpwang@umn.edu; yjiang@ustb.edu.cn

Section I: The calculation of the number of ds-DNA attached on per MNPs

The hysteresis loops of HM and LM MNPs were measured by VSM. And the moment of per-MNPs was fitted by the langevin and hyperbolic tangent functions. The moments of per-MNPs are 1.24×10^{-16} and 9.43×10^{-16} emu for LM and HM MNPs, respectively.





So the total number of MNPs in the solution ($N_{\text{total-MNPs}}$) can be expressed as:

$$N_{total-SNPs} = \frac{M_{total}}{M_{per-MNPs}}$$

Where M_{total} is the total moment of MNPs and $M_{\text{per-MNPs}}$ is the moment of per-MNPs.

The number of ds-DNA on per-MNPs ($N_{\text{ds-DNA}}$) can be expressed as follow:

$$N_{ds-DNA} = \frac{C_{ds-DNA} \times V \times N_A}{N_{total-MNPs}}$$

Where $C_{\text{ds-DNA}}$ is the concentration of ds-DNA, V is the volume of solution and N_A is the Avogadro constant.

Section II: Theoretical relation of ds-DNA fraction and temperature

During the hyperthermia process, the two released ss-DNA (A and A') quickly reach an equilibrium with ds-DNA (AA'). This reaction is expressed in **Equation S1**.

$$A + A' \Leftrightarrow AA' \tag{S1}$$

The thermodynamic equations of this process can be expressed as **Equation S2**.

$$\Delta G = \Delta H - T\Delta S$$

$$\Delta G = -RT \ln K_{eq}$$

$$K_{eq} = e^{\left(\frac{\Delta S}{R} - \frac{\Delta H}{RT}\right)} \tag{S2}$$

Where the ΔG, ΔH and ΔS are the Gibbs energy, enthalpy change and entropy change, respectively.

The K_{eq} also can be expressed as **Equation S3**.

$$f = \frac{2C_{DS}}{C_T} = \frac{C_T - 2C_{SS}}{C_T} = 1 - \frac{2C_{SS}}{C_T}$$

$$C_{SS} = \frac{(1-f)C_T}{2}$$

$$K_{eq} = \frac{[AA']}{[A][A']} = \frac{2f}{(1-f)^2 C_T} \tag{S3}$$

Where C_{SS} is the concentration of ss-DNA, C_{DS} is the concentration of ds-DNA, C_T is the concentration of total DNA strand and *f* is the fraction of ds-DNA.

The concentrations of the reaction products are related by the equilibrium constant.

Combined Equation S2 and S3, the temperature can be written in function of the fraction of ds-DNA (*f*), as shown in **Equation S4.**

$$T(f) = \frac{\Delta H}{\Delta S - R\ln\left[\frac{2f}{(1-f)^2 C_T}\right]} \tag{S4}$$

The exact thermodynamic parameters are calculated based on the nearest neighbor principle, as shown in **Table S1**

ΔH (kcalmol^{-1})	ΔS (calK^{-1}mol^{-1})	R (calK^{-1}mol^{-1})	C_{T_LM} (molL^{-1})	C_{T_HM} (molL^{-1})
-235.1	-614.6	1.987	1.58E-5	8E-5

Table S1. The thermodynamic parameters used in the calculation