

# Size-tunable NaGdF<sub>4</sub> nanoparticles as T<sub>2</sub> contrast agents for high-field magnetic resonance imaging

Zhigao Lu,<sup>†,‡</sup> Ruijun Deng,<sup>†,‡</sup> Mingming Zhen,<sup>†,‡,\*</sup> Xue Li,<sup>†,‡</sup> Toujun Zou,<sup>†</sup> Yue  
Zhou,<sup>†,‡</sup> Mirong Guan,<sup>†</sup> Ying Zhang,<sup>†,‡</sup> Yuqing Wang,<sup>§</sup> Tong Yu,<sup>†,‡</sup> Chunying Shu,<sup>†,‡</sup>  
and Chunru Wang,<sup>†,‡,\*</sup>

<sup>†</sup>Beijing National Laboratory for Molecular Sciences, Laboratory of Molecular Nanostructure and Nanotechnology, CAS Research/Education Center for Excellence in Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China.

<sup>‡</sup>University of Chinese Academy of Sciences, Beijing 100049, China.

<sup>§</sup>CAS key laboratory for Biomedical Effects of Nanomaterials and Nanosafety, National center for nanoscience and Technology of china, NO.11 Zhongguanyuan Beiyitiao, Beijing, 100190, china.

E-mail: crwang@iccas.ac.cn, zhenmm@iccas.ac.cn, Tel: 86-10-62652120;

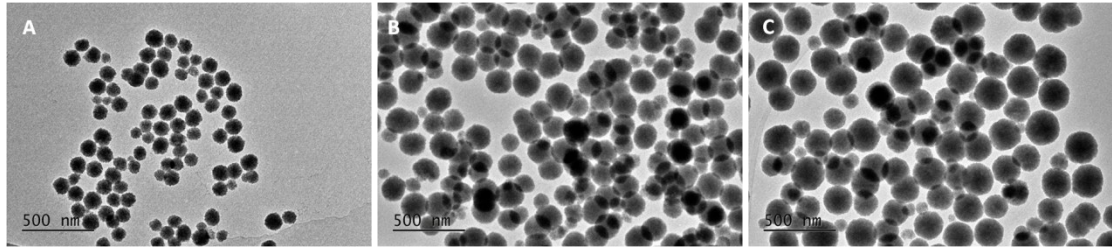


Figure S1. TEM images of NaGdF<sub>4</sub> NPs, samples 1 ( A ) , samples 2 ( B ) , and samples 3 ( C ) .

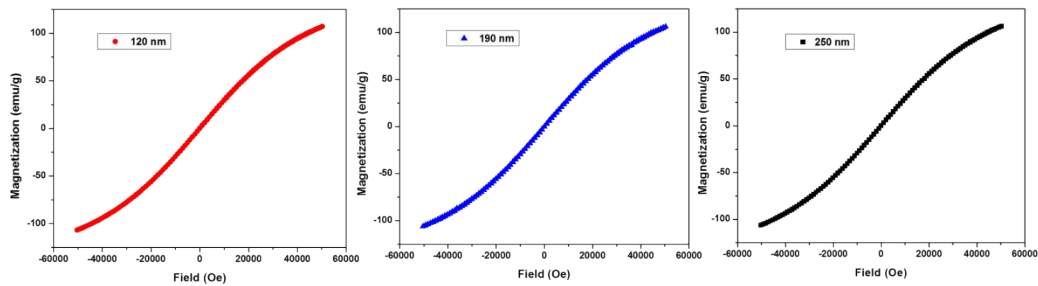


Figure S2 Mass magnetization of different size of NaGdF<sub>4</sub>@SiO<sub>2</sub> NPs obtained using a SQUID magnetometer. red line: 120 nm, blue line 190 nm, black line 250 nm

Particle size (nm)	$r_1/[Gd^{3+}](mM^{-1}S^{-1})$		$r_2/[Gd^{3+}](mM^{-1}S^{-1})$		$r_2/r_1$	
	0.5 T	7 T	0.5 T	7 T	0.5 T	7 T
120	1.422	0.746	4.359	129.7	3.06	173.8
190	0.548	0.471	5.754	142.9	10.5	303.4
250	0.393	0.272	8.553	159.6	21.76	586.8

Table S1.  $r_1$  and  $r_2$  relaxivity and  $r_2/r_1$  values of NaGdF<sub>4</sub>@SiO<sub>2</sub> using 0.5 T and 7 T MRI scanner.

Particle size (nm)	0.5 T				7 T			
	$r_2/[Gd^{3+}]$ (mM <sup>-1</sup> S <sup>-1</sup> )	$r_2/M$ (mg/ml) <sup>-1</sup> S <sup>-1</sup>	$r_2/NP$ (mM <sup>-1</sup> S <sup>-1</sup> )	$r_2/r_1$	$r_2/[Gd^{3+}]$ (mM <sup>-1</sup> S <sup>-1</sup> )	$r_2/M$ (mg/ml) <sup>-1</sup> S <sup>-1</sup>	$r_2/NP$ (mM <sup>-1</sup> S <sup>-1</sup> )	$r_2/r_1$
120	4.359	17	$5.2 \times 10^7$	3.06	129.7	512	$1.56 \times 10^9$	173.8
190	5.754	22	$2.7 \times 10^8$	10.5	142.9	558	$6.81 \times 10^9$	303.4
250	8.553	33	$9.3 \times 10^8$	21.76	159.6	623	$1.73 \times 10^{10}$	586.8

Table S2.  $r_2$  relaxivity,  $r_2/M$ ,  $r_2/NP$  and  $r_2/r_1$  values of NaGdF<sub>4</sub>@SiO<sub>2</sub> using 0.5 T and 7 T MRI scanner.

## Relaxivity Calculation<sup>1</sup>

The concentration of Gd<sup>3+</sup> ions determined by ICP-MS in the stock solution was used to calculate the molecular mass of NaGdF<sub>4</sub> in the specimen using the ratio

$$m(\text{Gd})/m(\text{NaGdF}_4) = 0.6137$$

This was used to calculate the  $r_1/M$  (mass relaxivity) values

The NaGdF<sub>4</sub> NPs synthesized have Hexagonal closed pack (HCP)-crystal structure and the density of HCP NaGdF<sub>4</sub> 5.65g/cc was used to determine the mass of a NP, considering that the NPs are perfect spheres and their volume determined using

$$V = 4/3\pi R^3 \text{ (where R is the radius of the NP)}$$

Comparing the mass of single NP and the total mass determined from ICP-MS the total number of NPs (N) in the stock solution was determined and used to calculate the  $r_2/\text{NP}$  (Nanoparticle relaxivity)

1. N. J. J. Johnson, W. Oakden, G. J. Stanis, R. Scott Prosser and F. C. J. M. van Veggel, *Chem. Mater.*, 2011, **23**, 3714-3722.