

Supplementary Information

Defect density modulation in graphene quantum dots towards high magnetic resonance relaxivity

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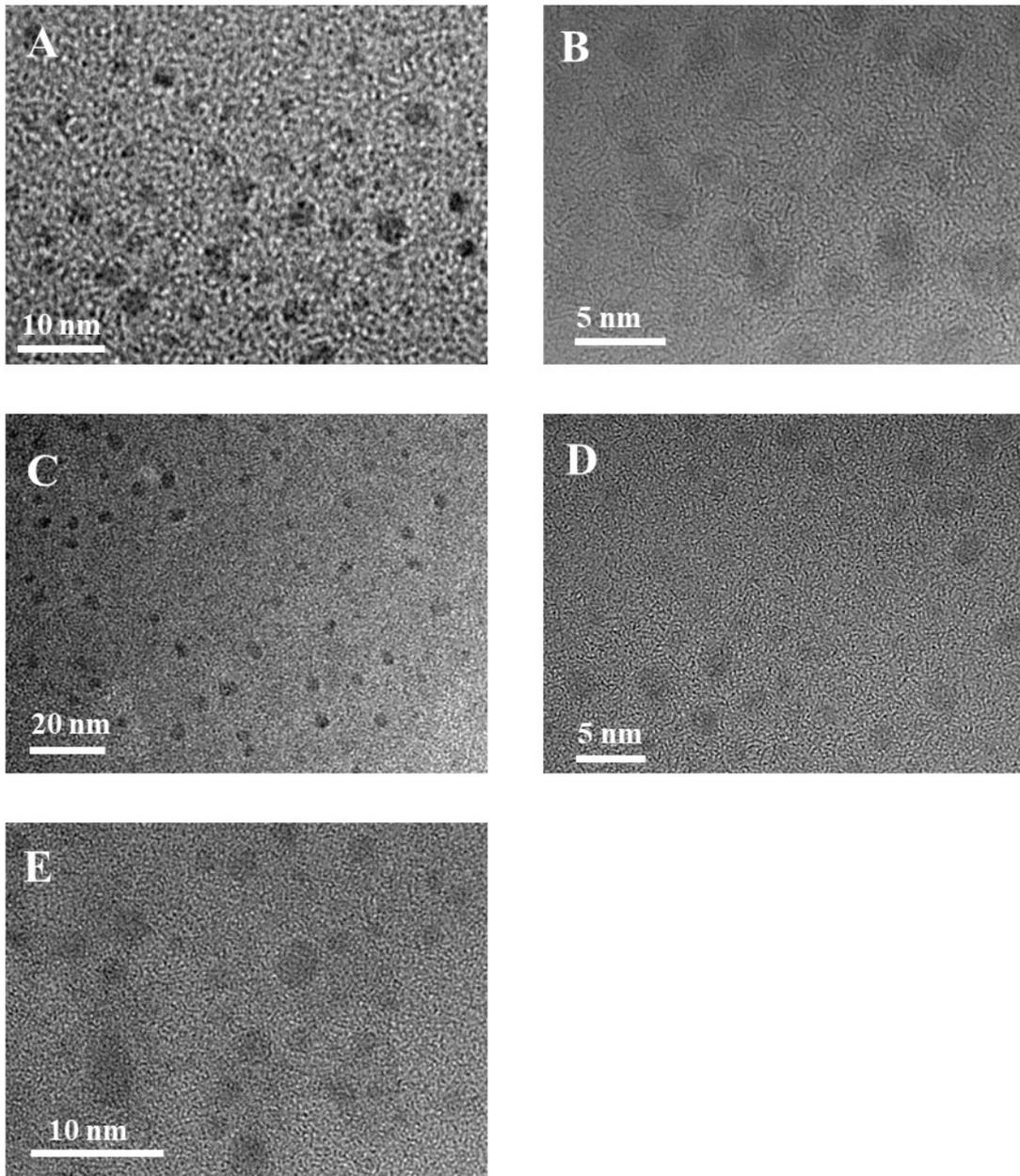


Figure S1. The TEM images of (A) $\text{Gd}^{3+}@\text{GQD-I}$, (B) $\text{Gd}^{3+}@\text{GQD-II}$, (C) $\text{Gd}^{3+}@\text{GQD-III}$, (D) $\text{Gd}^{3+}@\text{GQD-IV}$, and (E) $\text{Gd}^{3+}@\text{GQD-V}$.

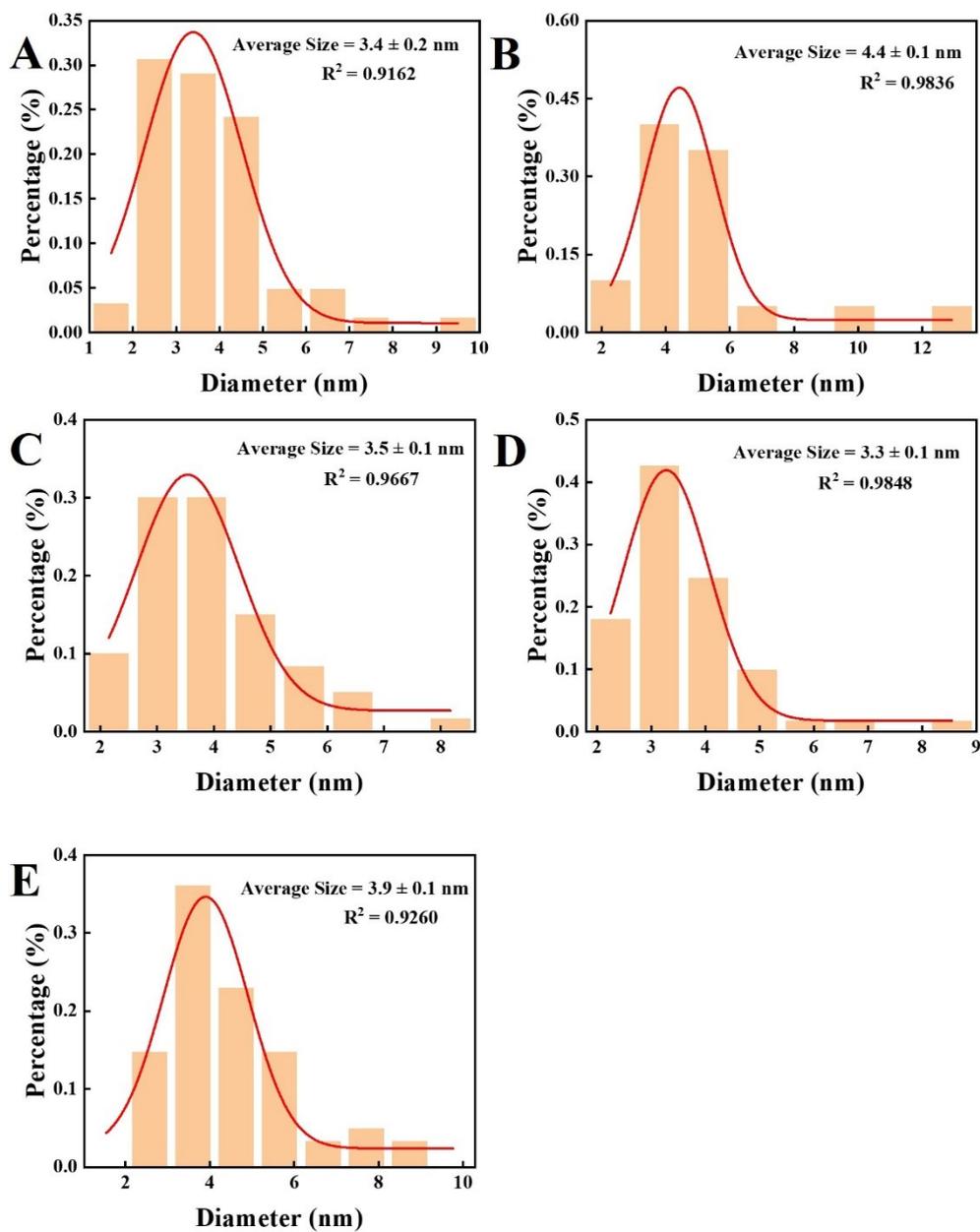


Figure S2. Histograms showing the particle size distributions of Gd³⁺@GQD-I (A), Gd³⁺@GQD-II (B), Gd³⁺@GQD-III (C), Gd³⁺@GQD-IV (D), and Gd³⁺@GQD-V (E) obtained by TEM.

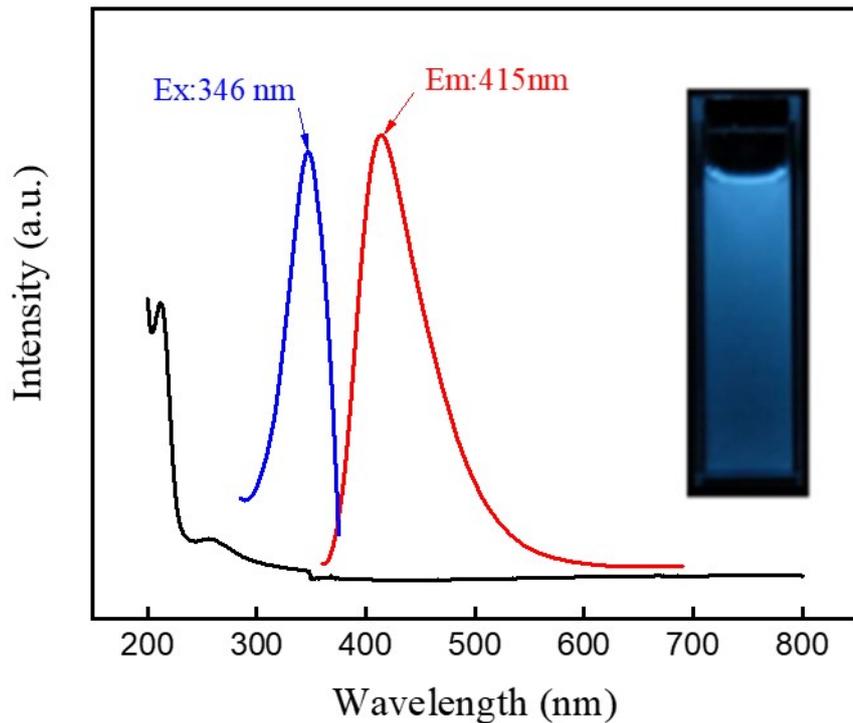


Figure S3. PL, PL excitation spectra, and ultraviolet visible (UV-Vis) absorption spectrum of Gd³⁺@GQD-V aqueous solution (inset: photograph of Gd³⁺@GQD-V in aqueous solution under 346 nm radiation). The optical excitation wavelength (λ_{ex}) of Gd³⁺@GQD-V is 346 nm, as proved by the PL excitation spectrum. The maximal emission wavelength (λ_{em}) is centered at 415 nm.

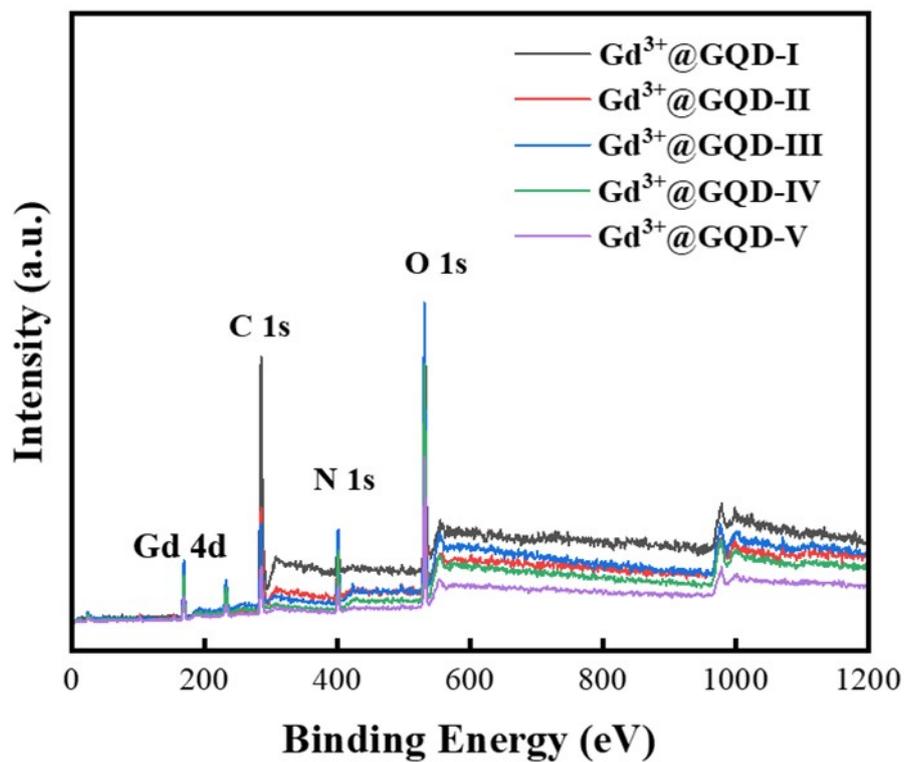


Figure S4. XPS survey map of Gd³⁺@GQD-I, Gd³⁺@GQD-II, Gd³⁺@GQD-III, Gd³⁺@GQD-IV, and Gd³⁺@GQD-V. It shows that all five types of Gd³⁺@GQDs have a C 1s peak at ca. 285.4 eV, N 1s peak at ca. 401.4 eV, along with an O 1s peak at ca. 532.3 eV. It also shows Gd 4d peaks at ca. 152.9 eV.

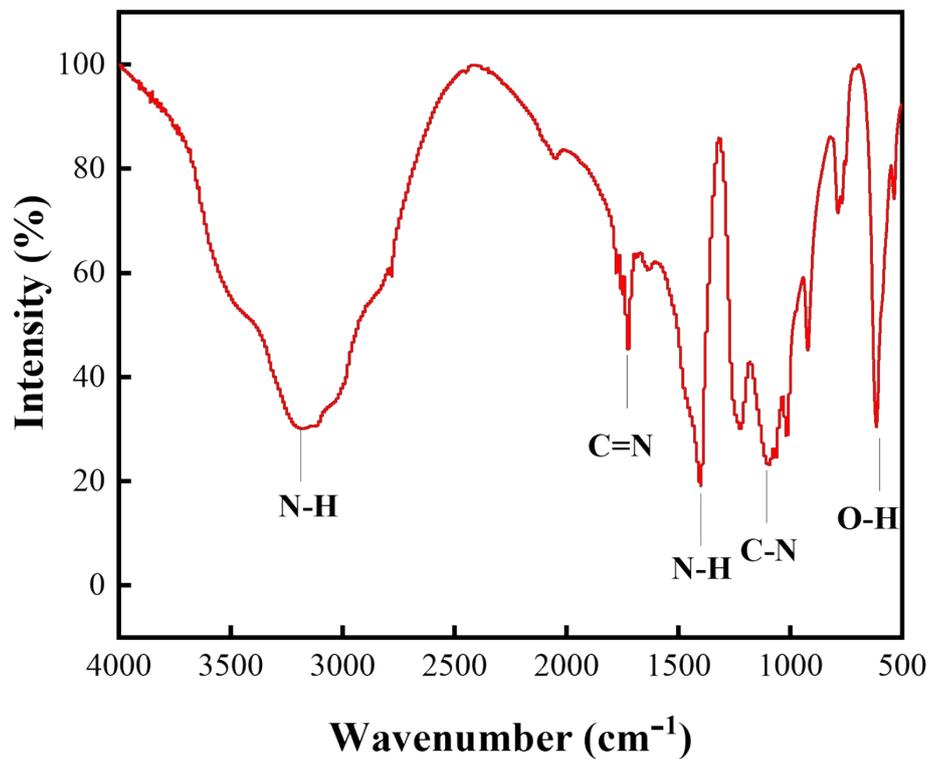


Figure S5. FT-IR spectrum of Gd³⁺@GQD-V.

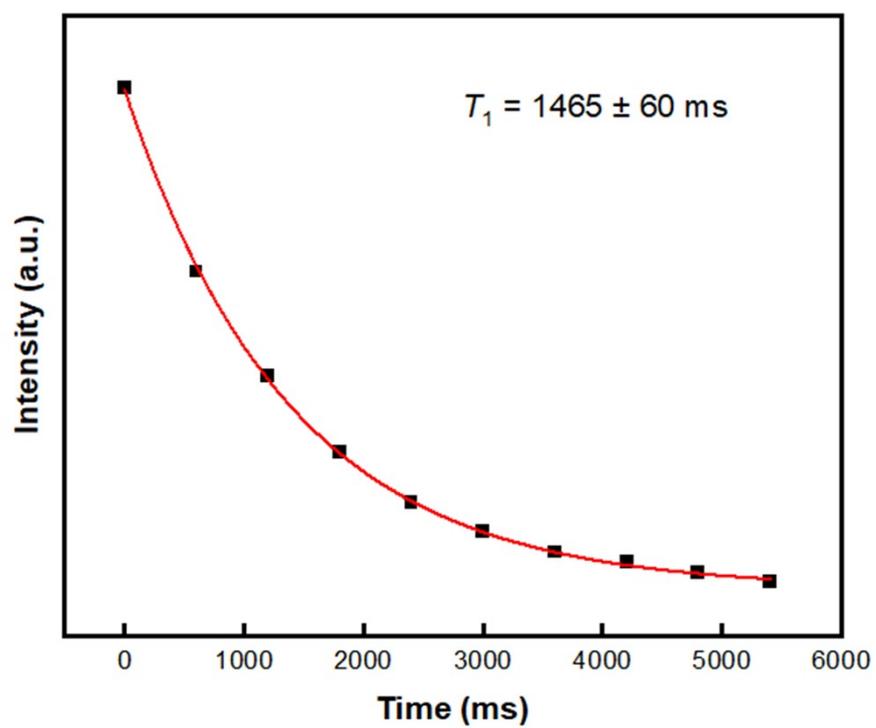


Figure S6. T_1 fitting of 0.04 mM Gd^{3+} @GQD-I. T_1 of 0.04 mM Gd^{3+} @GQD-I is 1465 ± 60 ms. T_1 was obtained by a single exponential fit.

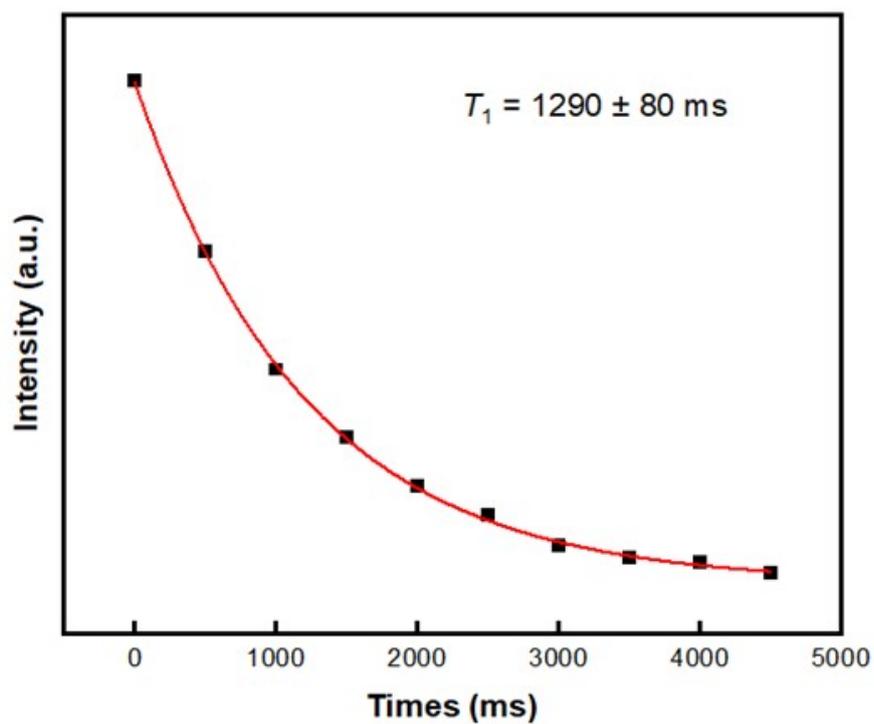


Figure S7. T_1 fitting of 0.04 mM Gd^{3+} @GQD-II. T_1 of 0.04 mM Gd^{3+} @GQD-II is 1290 ± 80 ms. T_1 was obtained by the single exponential fit.

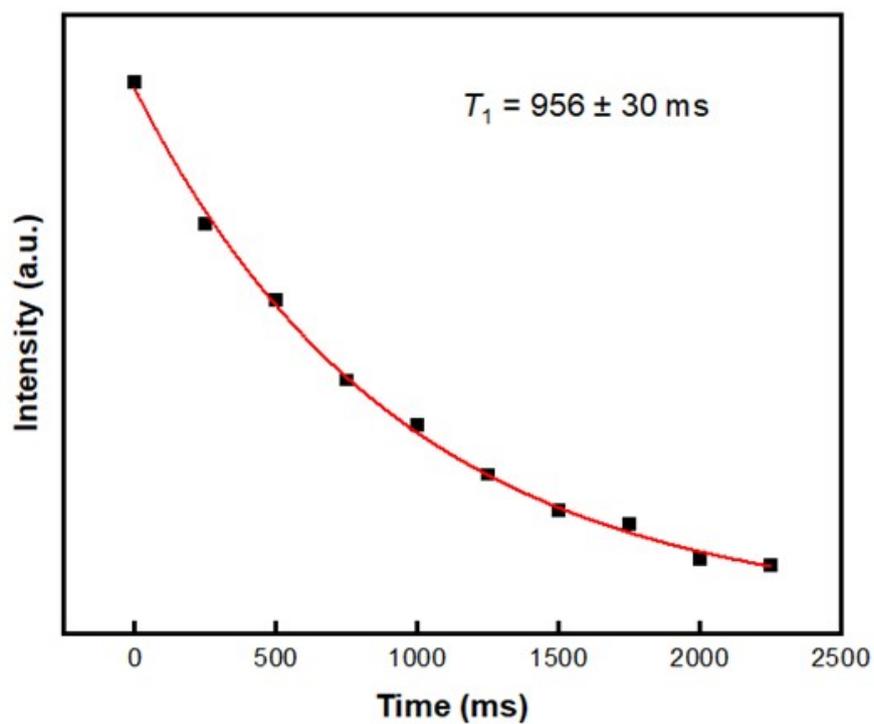


Figure S8. T_1 fitting of 0.04 mM Gd^{3+} @GQD-III. T_1 of 0.04 mM Gd^{3+} @GQD-III is 956 ± 30 ms. T_1 was obtained by the single exponential fit.

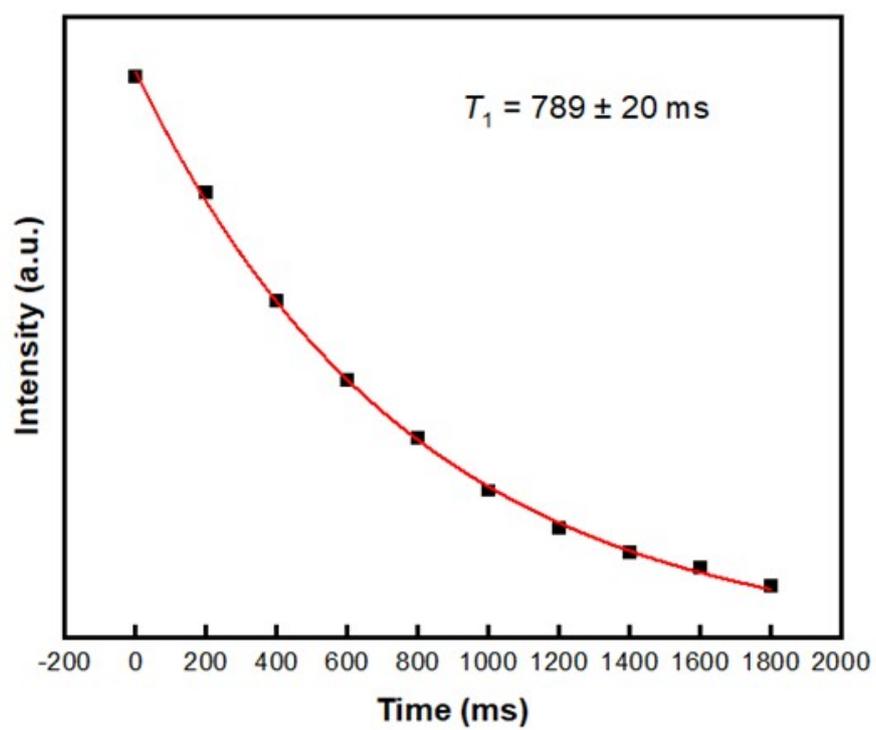


Figure S9. T_1 fitting of 0.04 mM Gd^{3+} @GQD-IV. T_1 of 0.04 mM Gd^{3+} @GQD-IV is 789 ± 20 ms. T_1 was obtained by a single exponential fit.

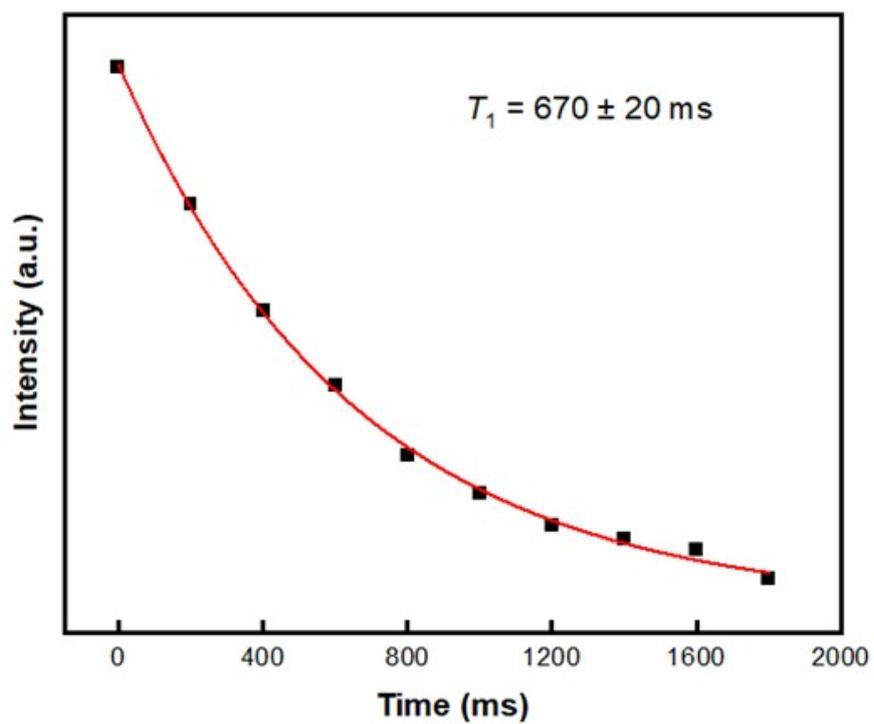


Figure S10. T_1 fitting of 0.04 mM Gd^{3+} @GQD-V. T_1 of 0.04 mM Gd^{3+} @GQD-V is 670 ± 20 ms. T_1 was obtained by a single exponential fit.

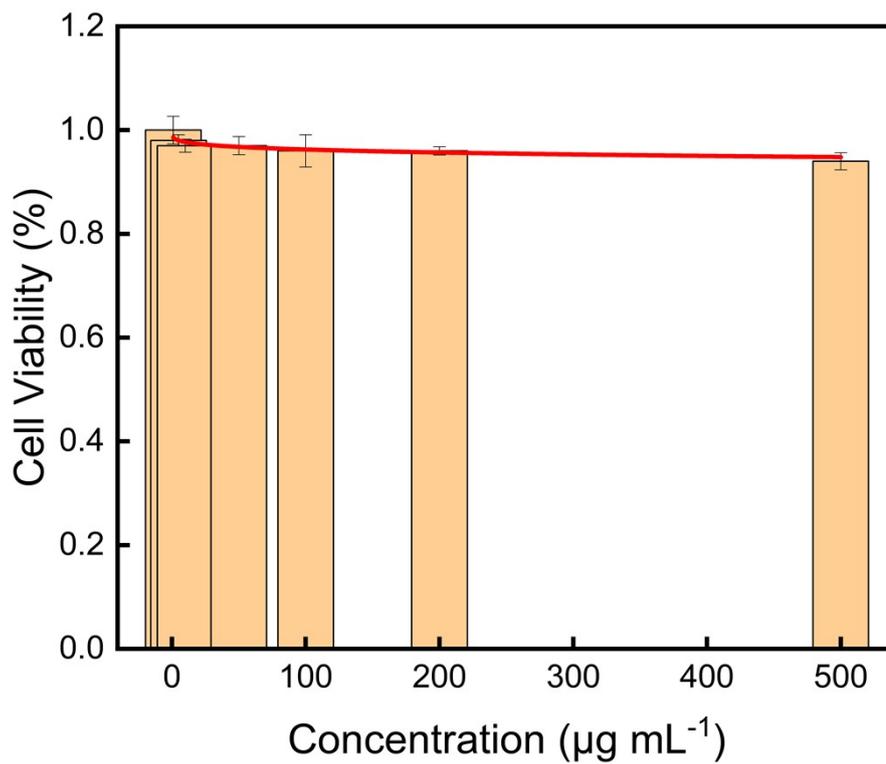


Figure S11. Viability of fibroblasts incubated for 48 h with $\text{Gd}^{3+}@GQD-V$ and fitted using the Hill model. Concentrations ranged from 1 to $500 \mu\text{g mL}^{-1}$. Error bars represent standard deviation of six independent experiments.

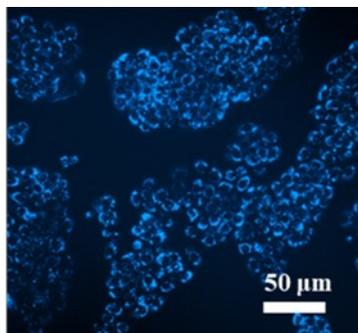


Figure S12. Fluorescence image of HaCaT cells after injecting with $100 \mu\text{g mL}^{-1}$ of $\text{Gd}^{3+}@GQD-V$ for 48 h.

Table S1. Detailed information on the precursors of GQDs

Precursor 1		Precursor 2		Product
Chemical	Content (mmol)	Chemical	Content (mmol)	
Melamine	7.9	Phloroglucinol	0.79	GQD-I
Melamine	7.9	1,2,4-Phenyltriphenol	0.79	GQD-II
Melamine	7.9	Catechol	0.79	GQD-III
Melamine	7.9	Resorcinol	0.79	GQD-IV
Melamine	7.9	Hydroquinone	0.79	GQD-V