Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.

Supporting Information

Grafting of Gd-DTPA onto MOF-808 with enhancing MRI performance for guiding photothermal therapy

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EXPERIMENTAL SECTION

Materials All purchased chemical reagents were directly used without further purification, and the secondary water used in the whole experiment was prepared by the ELGA water purification system (PURELAB Classic). Mesitylic acid (99%) and Diethylenetriamine pentaacetic acid (98%, DTPA) were purchased from Sigma-Aldrich company. Zirconium oxychloride octahydrate (98%) was bought from Jiangsu Aikang biomedical research and Development Co., Ltd. And Gadolinium nitrate hexahydrate (99%, $Gd(NO_3)_3 \cdot 6H_2O$) was purchased from Acros company, hydrochloric acid and Sodium hydroxide (NaOH) were bought from Shanghai Runjie chemical reagent company, Aniline (99%) was purchased from Adamas company. N. N-dimethylformamide (99%, DMF), formic acid, and methanol were all obtained from Sinopharm Chemical Reagent Co., Ltd.

Characterization The crystalline structures data of the samples were collected by D/MAX2000 X-ray powder diffractometer, and the scanning range was 3-35°. The scanning electron microscope (SEM) and transmission electron microscope (TEM) images were performed by Hitachi S-4800 and JEM-2010F respectively. Fourier transform infrared (FTIR) characterization was conducted on Nicolet Avatar 370 FT-IR instrument with wavenumbers of 400-4000 cm^{-1}. The UV absorption curve of the solution was obtained by UV/VIS spectrophotometer (DU730). The hydrated particle size and potential of nanoparticles were obtained on a dynamic light scattering particle size potential analyzer (ZEN3690). The amount of metallic element was measured by inductively coupled plasma atomic emission spectrometry (Vista MPX ICP).

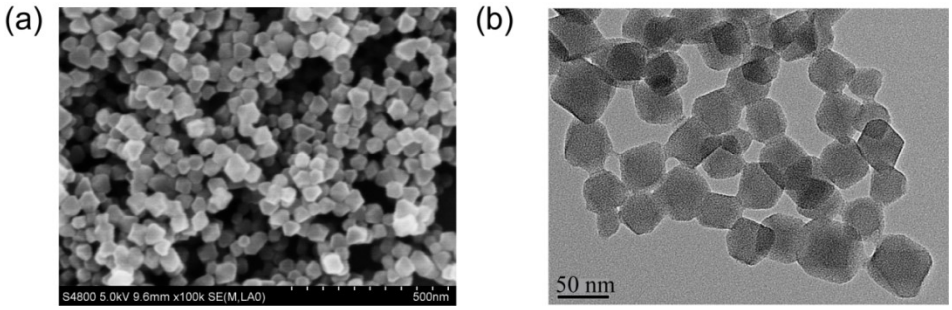

Fig. S1 (a) SEM and (b) TEM of MOF-808.

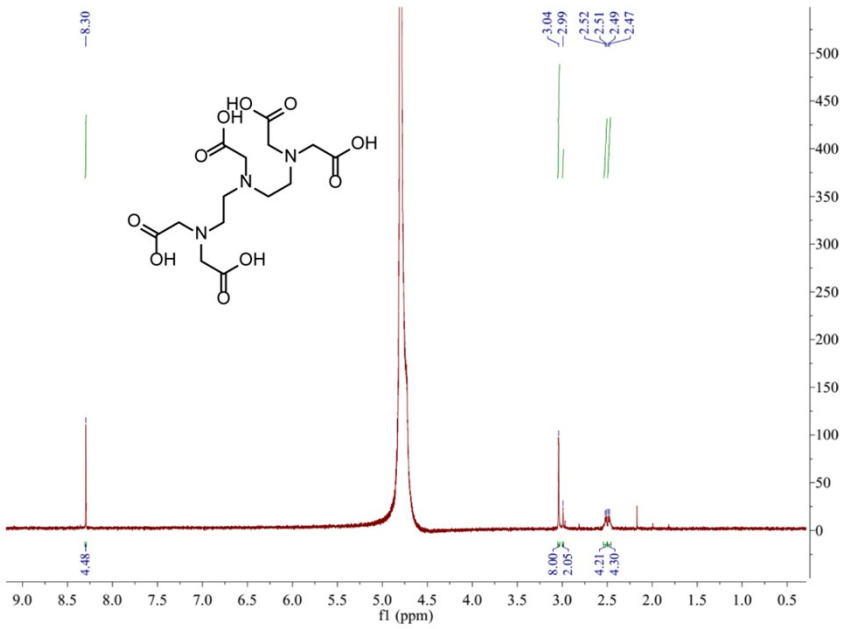

Fig. S2 ^{1}H nuclear magnetic resonance (NMR) spectrum of MOF-808-DTPA. The illustration shows the structure of DTPA.

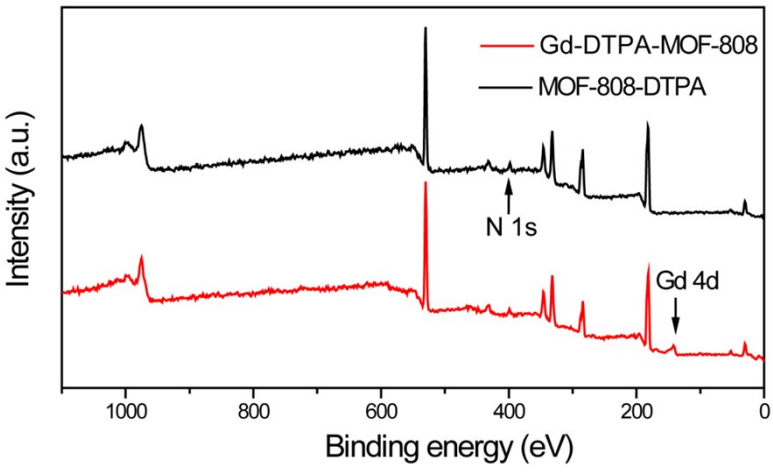

Fig. S3 XPS diagram of Gd-DTPA-MOF-808 and MOF-808-DTPA.

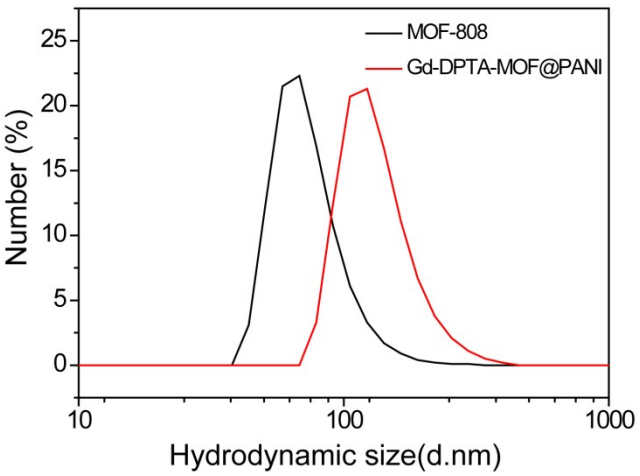

Fig. S4 Hydrated particle size distribution of MOF-808 and Gd-DTPA-MOF-808@PANI.

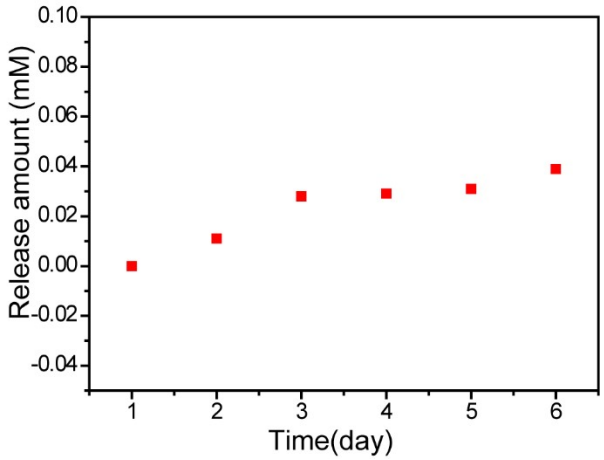

Fig. S5 The amount of Gd ion released from MOF-808-DTPA-Gd@PANI in aqueous solution was tracked for 6 days (with 50 mg of Gd-DTPA-MOF-808@PANI immersed in 5 mL of water).

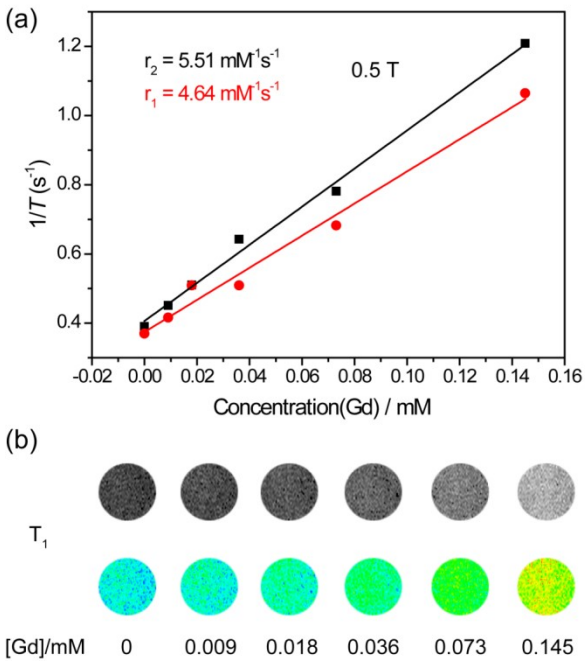

Fig. S6 (a) The relaxation rate and (b) MR imaging of Gd-DTPA.

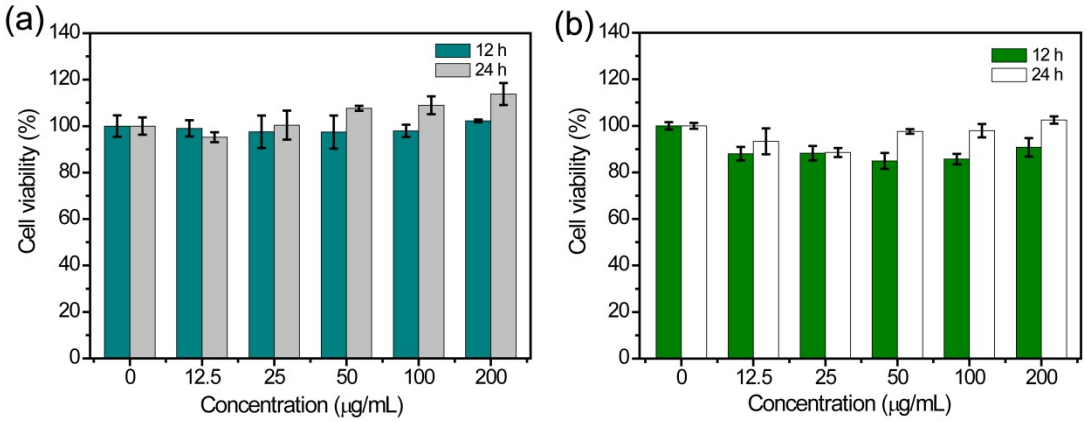

Fig. S7 The (a) HUVEC and (b) 4T1 cell viability treated with varying concentrations of Gd-DTPA-MOF-808@PANI for 12 and 24 h were evaluated by MTT assay.

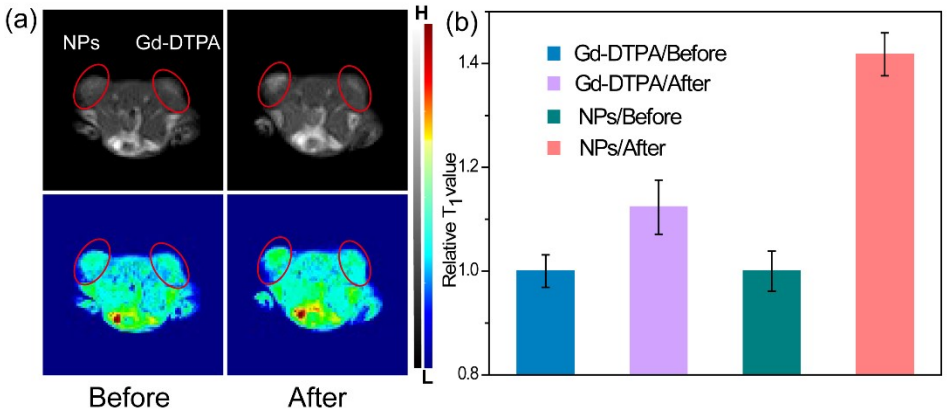

Fig. S8 (a) T_1 imaging (0.5 T) of mice after injecting Gd-DTPA-MOF-808@PANI into the tumor on the left side and commercial Gd-DTPA on the right side. The red circle was the site of the tumor. (b) The relative T_1 signal value of the corresponding tumor area. NPs was refer to Gd-DTPA-MOF-808@PANI.

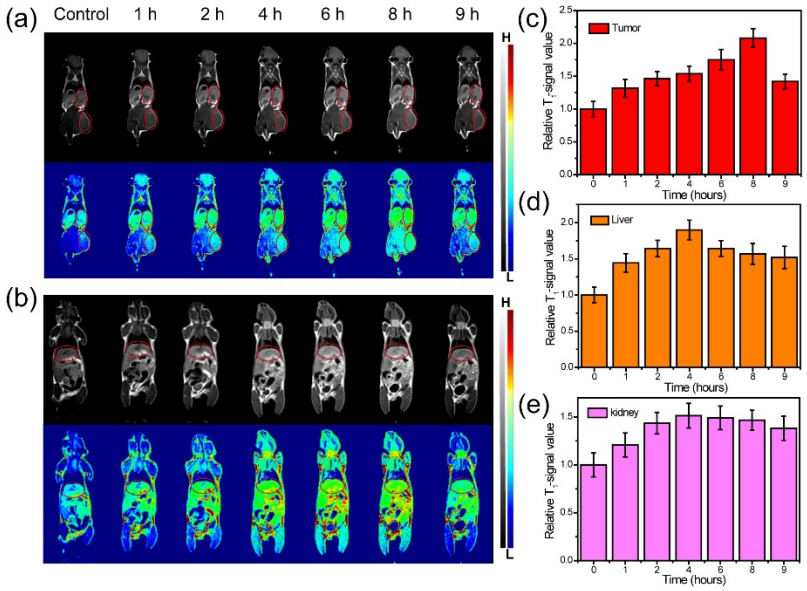

Fig. S9 (a, b) MR imaging on the coronal plane of 4T1 mice in different periods after injecting Gd-DTPA-MOF-808@PANI (0.5 T). Histogram of T_1 signal values at (c) tumor, (d) liver, and (e) kidney corresponding to MR imaging.

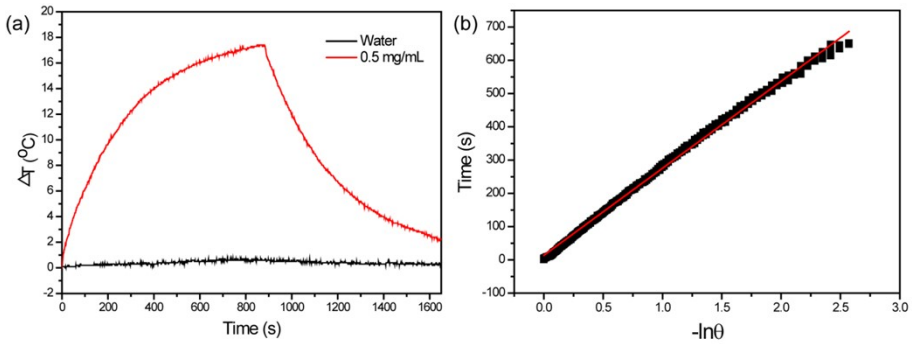

Fig. S10 (a) The temperature rise and fall curve of Gd-DTPA-MOF-808@PANI (0.5 mg mL^{-1}) irradiated with 808 nm laser (1.0 W cm^{-1}). (b) The photothermal conversion fitting curve of Gd-DTPA-MOF-808@PANI (0.5 mg mL^{-1}).

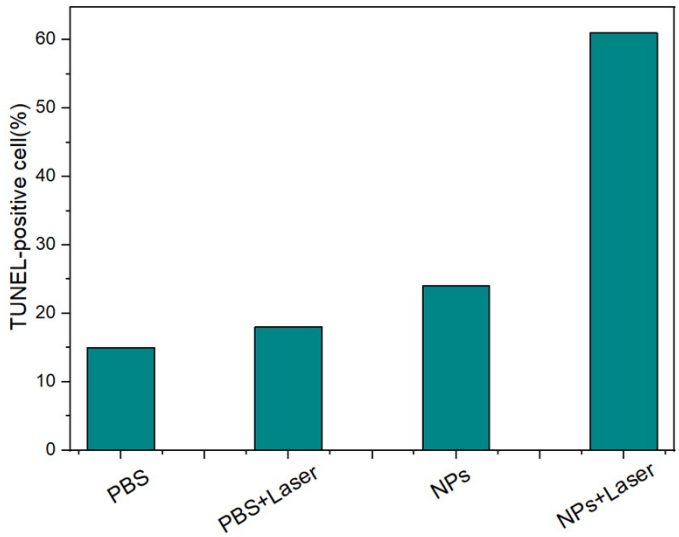

Fig. S11 Statistics of tumor cell mortality in different groups in TUNEL staining.

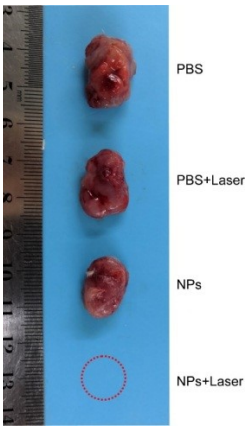

Fig. S12 Photos of tumors removed after 16 days of treatment in mice.