Supporting Information for

Graphitic-N-doped graphene quantum dots for photothermal eradication of multidrug-resistant bacterial in the second near-infrared window

Bijiang Geng,*a† Yuan Li,† Jinyan Hu,a Yuanyuan Chen,b Junyi Huang,b Longxiang Shen,c Dengyu Pan* a and Ping Li* b

a School of Environmental and Chemical Engineering, Shanghai University, Shanghai 200444, China.
b School of Life Sciences, Shanghai University, Shanghai 200444, China.
c Department of Orthopedic Surgery, Shanghai Jiao Tong University affiliated Sixth People’s Hospital, Shanghai 200233, China

Fig. S1 The photographs of N-GQD solution stored for 90 days.

Fig. S2 The absorption spectrum of GQDs without N doped.
**Fig. S3** Zeta potential of N-GQDs (200 µg/mL).

**Fig. S4** The high-resolution O 1s spectrum of N-GQDs.

**Fig. S5** (a) PL spectra of N-GQDs excited at different wavelengths varied from 350 to 400 nm. (b) Dependence of PL intensity on pH values. (c) Photostability test under 5 h continuous radiation using a 100 W xenon lamp.
Fig. S6 (a, b) Plot of temperature change ($\Delta T$) over a period of 300 s versus different concentrations of N-GQDs under irradiation with an 808 (a) and 1064 nm (b) laser irradiation at the power density of 0.4 and 1.0 W/cm$^2$, respectively. (c, d) Plot of temperature change ($\Delta T$) over a period of 300 s versus 808 (c) or 1064 nm (d) laser power density.

Fig. S7 Temperature elevation of N-GQDs (200 $\mu$g/mL) stored for different times (0, 1, and 7 days) under 1064 nm (1.0 W/cm$^2$) laser irradiation.
Fig. S8 Survey XPS spectrum, High-resolution C 1s, N 1s, and O 1s spectra of N-GQD\textsubscript{600}.

Fig. S9 Survey XPS spectrum, High-resolution C 1s, N 1s, and O 1s spectra of N-GQD\textsubscript{10000}.
Fig. S10 (a) NIR absorption spectra of three N-GQD samples at the same concentration (200 µg/mL). (b, c) The photothermal conversion efficiency measurements of three N-GQD samples at the same concentration (200 µg/mL). Photothermal effect of the three N-GQD solution exposed to the 808 nm laser at 0.4 W/cm². The lasers were shut off after 300 s irradiation. Plot of cooling time versus negative natural logarithm of the temperature driving force obtained from the cooling period after the 808 nm irradiation. (d) Proposed formation mechanism of \( F \) centers at graphitic N sites, where N atoms donate one excess electron and form \( N^+ \) cations to trap the electron with a large binding energy. (e) Defect energy levels of doped graphitic N as a \( F \) center within the wide band gap of N-GQDs and possible optical transitions from the HOMO level to the defect level and from the singly-occupied defect level to the LUMO level under the NIR excitation.

Fig. S11 (a) In vitro cytotoxicity of BEAS-2B cells after receiving treatments with N-GQDs at varied concentrations. (b) Hemolytic percentages of RBCs treated with different concentrations of N-GQD
solution for 3 h.

**Fig. S12**  (a, b) Photographic images of the colonies (a) and the survival rate (b) of *S. aureus* after receiving treatments with varied concentrations of N-GQD aqueous solution without or with 808 (0.4 W/cm²) or 1064 nm laser (1.0 W/cm²) irradiation for 5 min.  (c) Biomass quantification of *S. aureus* biofilms in (d) by measurement of absorbance at 595 nm.  (d) Image of crystal violet staining of *S. aureus* biofilm on glass slides.  (e) Live (green fluorescence, SYTO9) and dead (red fluorescence, PI) staining of *S. aureus* under various treatments.  (f) SEM images of *S. aureus* after receiving various treatments.
**Fig. S13** (a, b) Photographic images of the colonies (a) and the survival rate (b) of *E. coli* after receiving treatments with varied concentrations of N-GQD aqueous solution without or with 808 (0.4 W/cm$^2$) or 1064 nm laser (1.0 W/cm$^2$) irradiation for 5 min. (c) Biomass quantification of *E. coli* biofilms in (d) by measurement of absorbance at 595 nm. (d) Image of crystal violet staining of *E. coli* biofilm on glass slides. (e) Live (green fluorescence, SYTO9) and dead (red fluorescence, PI) staining of *E. coli* under various treatments. (f) SEM images of *E. coli* after receiving various treatments.

**Fig. S14** Wound area from the four groups at different time points during the therapeutic process.
**Fig. S15** Statistic analysis of the colony numbers on the LB plate from each group (Group 1: Control; Group 2: NIR; Group 3: N-GQD; Group 4: N-GQD + NIR).

**Fig. S16** Body weight of the mice in each group during the therapeutic process.