Broad-Spectrum Light-Responsive N-Doped Graphene Quantum Dots for Efficient Photocatalytic Generation of Hydroxyl Radicals and Antibacterial Applications

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Calculation of OH yield

To determine OH radical production, we first established a linear relationship between the concentration of 2hTA and its PL intensity under 310 nm excitation, as shown in Figure S1a. The result was:

$$[2hTA] = 1.5 \times 10^{-5} \times Intentisity - 0.52$$

Using this calibration, the OH radical concentration in Samples (1)-(4) was calculated from their corresponding PL intensities. The net OH radical concentration from the H_2O_2-to-OH conversion by N-GQDs was then determined by subtracting the Samples (2) and (3) from the total OH concentration in Sample (1), as expressed by:

$$[OH]_{H_2O_2-to-OH\ conversion\ by\ N-GQDs} = [OH]_{Sample\,(1)} - [OH]_{Sample\,(2)} - [OH]_{Sample\,(3)}$$

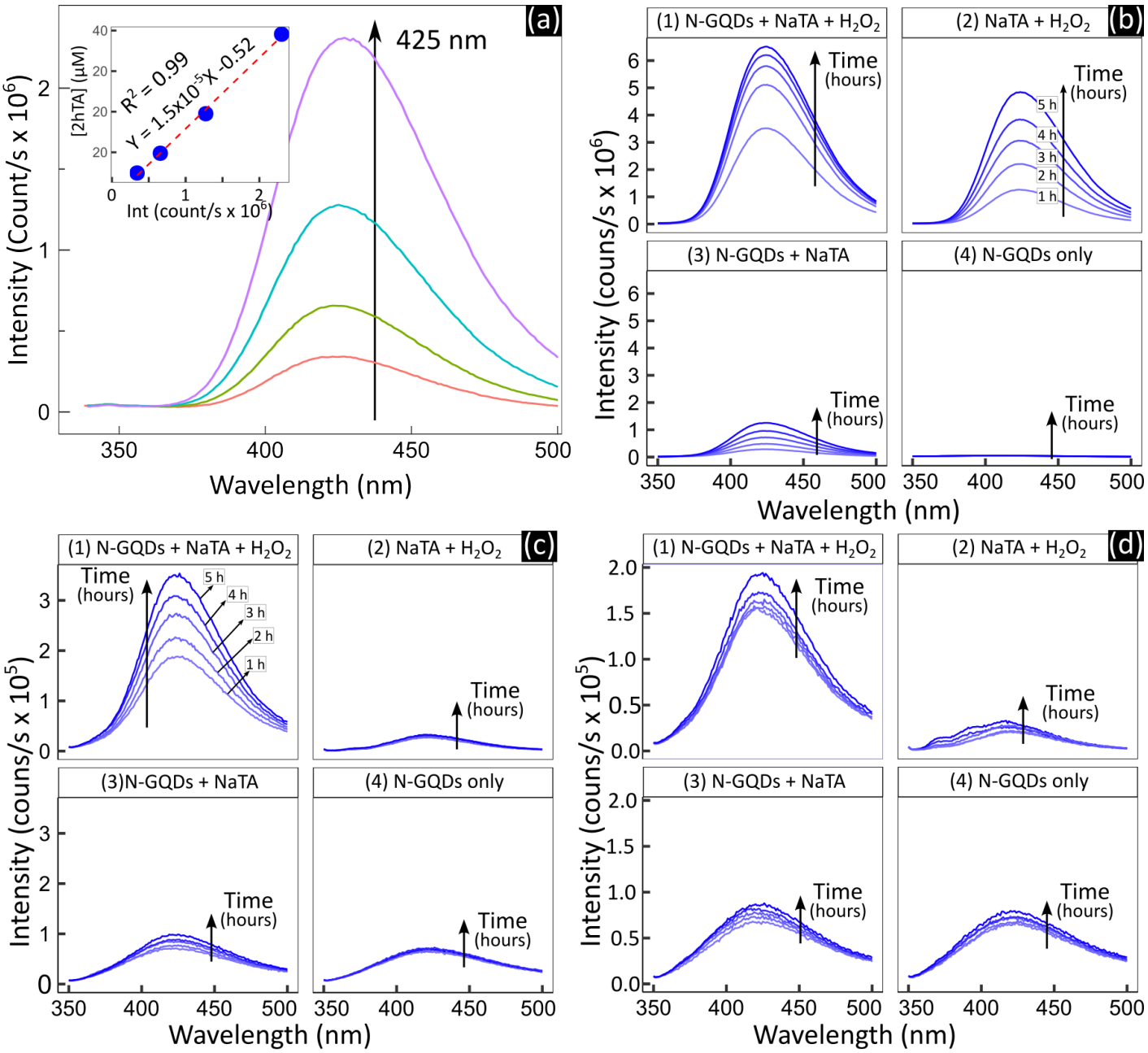

Figure S 1 (a) PL spectra of 2-hydroxyterephthalic acid (2hTA) solutions at different concentrations, with inset showing the linear regression between 2hTA concentration and PL intensity. (b-d) Time evolution of PL spectra (excitation at 310 nm) of solutions under UVA, green, and red light irradiation, respectively.

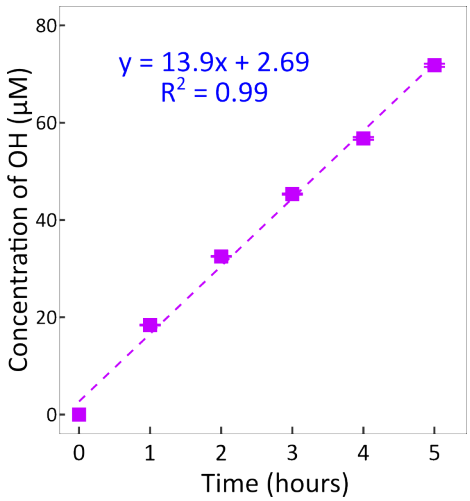

Figure S 2 Time-evolution of OH radical concentration generated in solution of NaTA + H_2O_2 under UVA illumination.The result was calculated from the PL spectra in Figure S1b. The concentration of OH radicals increases linearly with time, following the equation Y = 13.9X + 2.69 (R^2 = 0.99), indicating a steady generation rate of $\sim$ 13.9 μM.h^{-1}.

Table S 1 Summary of the interpretation of N 1s and C 1s spectra of N-GQDs[1–4].

Peaks	Core level binding energy (eV)	FWHM (eV)	G-L (0-1)
——————— C_{1s} ———————			
Graphitic carbon	284.3 - 284.8	1.2 - 2.0	0 - 0.3
C_{sp3}-N in pyridinic, pyrrolic forms	284.8 - 285.5	1.2 - 2.0	0 - 0.3
C-O, C_{sp3}-N, C-OH	285.6 - 286.5	1.4 - 2.4	0 - 0.2
Carbonyl (C=O)	286.5 - 288.0	1.4 - 2.4	0 - 0.2
Carboxyl (COOH)	288.0 - 289.2	1.4 - 2.4	0 - 0.2
Shake-up	291.0 - 294.0	1.4 - 2.4	0 - 0.2
——————— N_{1s} ———————			
Pyridinic - N	397.8 - 398.8	1.4 - 2.0	0 - 0.2
Pyridone/C_3N_4/amine	399.6 - 399.9	1.4 - 2.0	0 - 0.2
Pyrrolic-N	399.9 - 400.7	1.4 - 2.0	0 - 0.2
Graphitic-N	401.2 - 401.8	1.4 - 2.0	0 - 0.2
Nitrogen oxide	402.2 - 404.2	1.4 - 2.0	0 - 0.2

Table S 2 The volume ratio of Staphylococcus aureus, N-GQDs, and H_2O_2 in one mL sample. The H_2O_2 stock solution was diluted and added to achieve final concentrations ranging from 10^{-1} to 0.1 M as designed.

Samples	SA density, N-GQDs, and H_2O_2
Control	225 μL SA 10^6 CFU.mL^{-1} + 775 μL H_2O
N-GQDs control	225 μL SA 10^6 CFU.mL^{-1} + 775 μL N-GQDs
H_2O_2 alone	225 μL SA 10^6 CFU.mL^{-1} + 770 μL H_2O + 25 μL H_2O_2
N-GQDs + H_2O_2	225 μL SA 10^6 CFU.mL^{-1} + 770 μL N-GQDs + 25 μL H_2O_2

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