Supporting Information

The Multifunctional Prussian Blue/Graphitic Carbon Nitride Nanocomposites for Fluorescence Imaging-Guided Photothermal and Photodynamic Combination Therapy

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Experimental Section

Characterization

Transmission electron microscopy (TEM) and scanning electron microscopy (SEM) were observed by JEOL 2010-H TEM and 7001F SEM (Tokyo, Japan). X-ray photoelectron spectra (XPS) and X-ray diffraction (XRD) were characterized by AXIS ULTRADLD X-ray photoelectron spectrometer (Kratos, Japan) and D8 Advance powder X-ray diffractometer (Bremen, Germany). Fourier transform infrared spectroscopy (FT-IR) of PBCN was recorded using a Nicolet iS5 spectrometer (Agilent Technologies, US). UV-vis absorption and fluorescence (FL) spectra of PBCN were determined by a UV-2600 spectrophotometer (Shanghai, China) and a Hitachi F-4500 spectrofluorometer (Tokyo, Japan), respectively. The laser used is an 808 nm multi-mode fiber coupled infrared semiconductor laser (LSR 808NL, Ningbo Yuanming Laser Technology Co., LtD., China,). Cell fluorescence images were observed by TCS SP5 II confocal laser scanning microscope (CLSM, Leica, Germany). The fluorescence quantum yield of PBCN was determined using a dimethyl sulfoxide solution of indocyanine green (QY_R=0.13) as the standard reference solution.

The Calculation of the Photothermal Conversion Efficiency

The photothermal conversion efficiency (η) was calculated according to the previously reported method [1-3] as follows:

$$\eta_{PBCN} = \frac{hA(T_{Max} - T_{Surr}) - Q_{Dis}}{I(1-10^{-A_{808}})} \quad (1)$$

where h represents the heat transfer coefficient, A represents the surface area of the cuvette, T_{Max} is the maximum temperature, and T_{Surr} is the initial temperature. Q_{Diss} is the heat associated with light absorption of the water. I is the power density of 808 nm laser, and A_{808} is the absorbance of PBCN at 808 nm.

$$hA = \frac{mC_w}{\tau_s} \quad (2)$$

Where m is the mass of the solution, and C_w is the specific heat capacity of water. τ is the heat transfer time constant of the system and defined as:

$$t = -\tau_s(ln\theta) \quad (3)$$

θ is a dimensionless parameter and defined as:

$$\theta = \frac{T - T_{Surr}}{T_{Max} - T_{Surr}} \quad (4)$$

Cytotoxicity assay of PBCN nanocomposites

The cytotoxicity of PBCN nanocomposites was evaluated using human MCF-7 cells via a 3-(4,5-dimethyl-2-thiazolyl)-2,5-diphenyl-2-H-tetrazolium bromide (MTT) assay. First, MCF-7 cells were seeded in 96-well plates and cultured with 5% CO_2 at 37 °C for 12 h. Then, the medium was replaced by fresh medium containing PBCN nanocomposites with different concentrations (0, 10, 25, 50,75, 100, 125, 150, and 200 μg/mL), and the cells were incubated for another 24 h. Next, each well was supplemented with MTT (10 μL, 1 mg/mL) and incubated for 4 h. The supernatant was removed and 150 μL dimethyl sulfoxide (DMSO) was added. Finally, a microplate reader was used to record the absorbance at 490 nm.

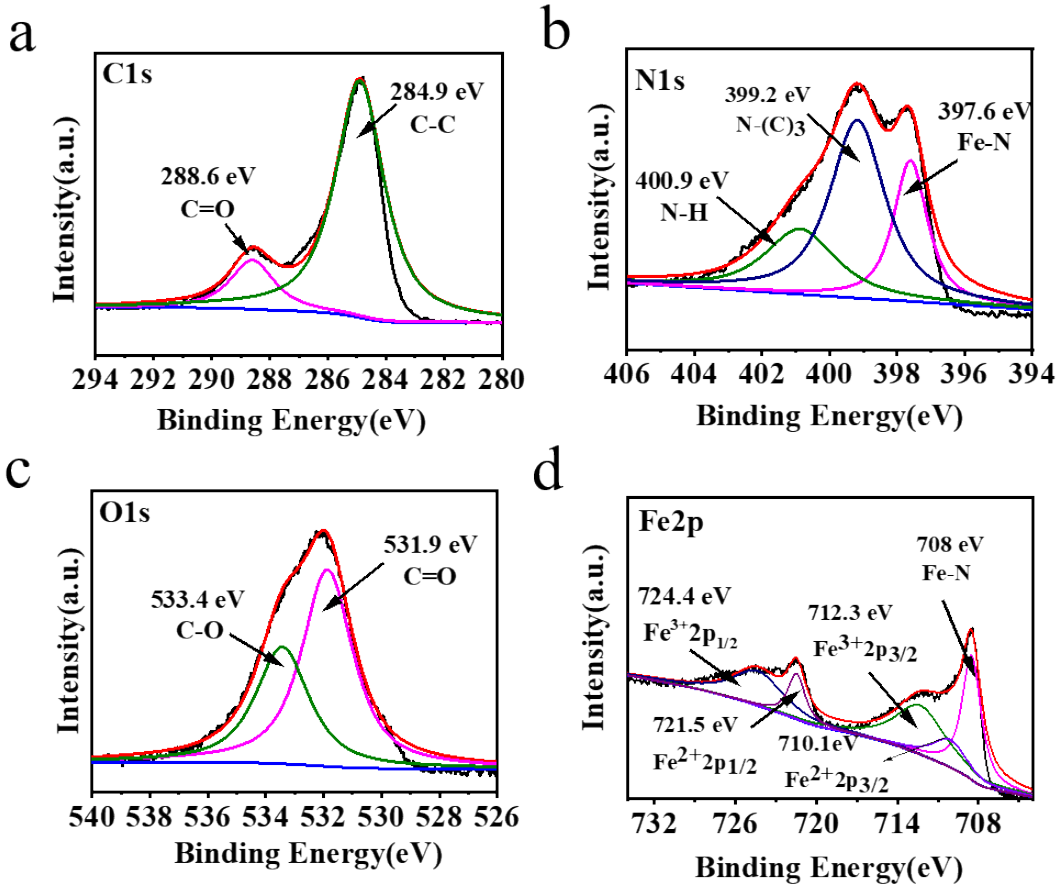

Fig. S1 The XPS spectrum of (a) C 1s, (b) N 1s, (c) O 1s, and (d) Fe 2p.

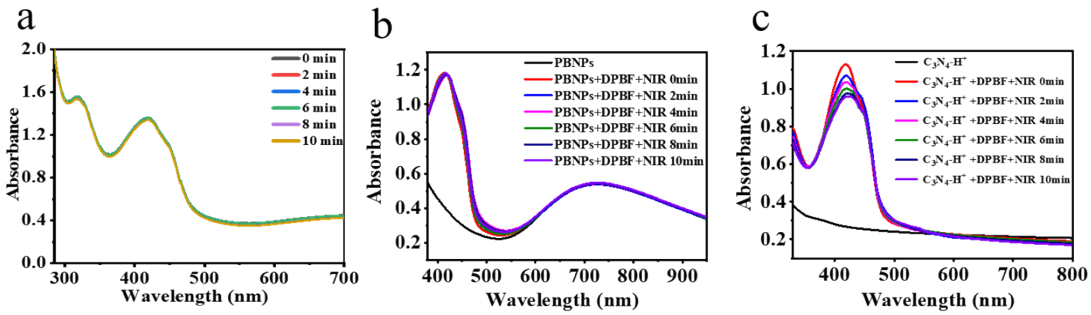

Fig.S2 The time-dependent degradation of DPBF at 425 nm caused by $^1O_2$ in (a) water, (b) PBNP solution, and (c) C_3N_4-H^+ solution after irradiation with 808 nm laser.

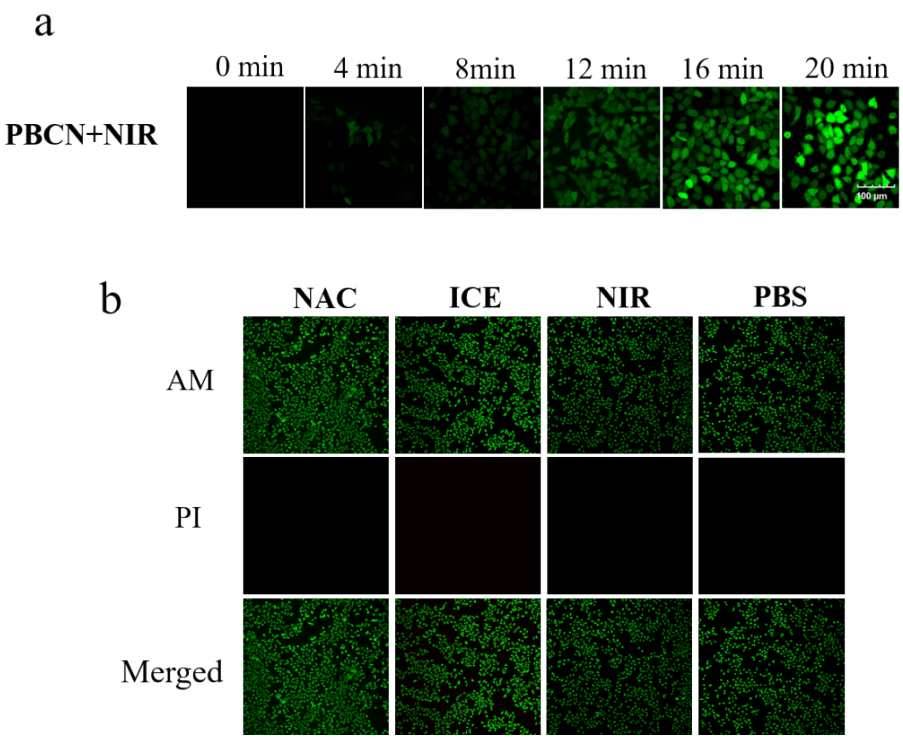

Fig.S3 (a) ROS production in MCF-7 cells using DCFH-DA probe with different irradiation times. (b) CLSM images of AM-PI stained MCF-7 cells with different treatments.

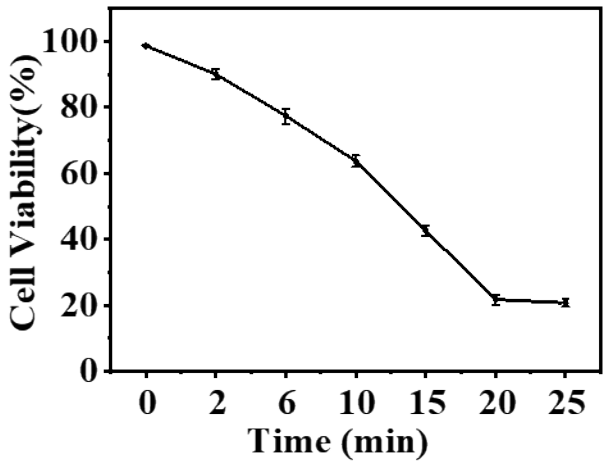

Fig.S4 Survival rate of MCF-7 cells incubating with 150 μg/mL PBCN and irradiating with 808 nm laser for different times.

References:

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2. B. Wang, G. Feng, M. Seifrid, M. Wang, B. Liu, *Angew. Chem. Int. Ed.,* 2017, **57**, 16063-16066.
3. C. Li, G. Jiang, J. Yu, W. Ji, L. Liu, P. Zhang, J. Du, C. Zhan, J. Wang and B. Z. Tang, *Adv Mater*, 2022, e2208229.