Supplementary Information

Construction of a Double Heterojunction between Graphite Carbon Nitride and Anatase TiO_2 with Co-exposed (101) and (001) Faces for Enhanced Photocatalytic Degradation

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(8 Pages, 9 Figures, 5 Table)

1. Preparation of g-C_3N_4/P25

1.15 g of g-C_3N_4 powder and 0.575 g P25 were added in a porcelain crucible containing 30 mL of ethyl alcohol and stirred until completely dry in the water bath at 80°C. And then move the crucible to a muffle furnace. At the heating rate of 3°C/min, the temperature was raised to 300°C and kept for 2 h. Finally, the g-C_3N_4/P25 powder was obtained.

2. The forbidden band width of synthetized photocatalysts were calculated by Tauc equation (1):

$$\alpha h v = A(hv - E_g)^n \tag{1}$$

Where α, hv, E_g, and A represent the absorption coefficient, incident photo energy, band gap energy, and absorption constant, respectively. Here, n = 2 due to anatase TiO_2 are indirect semiconductor materials.

3. The percentage of {001} and {101} facets can be calculated by equation (2-4):

$$S_{001} = 2a^2 \tag{2}$$

$$S_{001}\% = \frac{\cos\theta}{\cos\theta + (\frac{a}{b})^{-2} - 1} \tag{3}$$

$$S_{101}\% = 1 - S_{001}\% \tag{4}$$

Here θ is the theoretical value (68.3°) for the angle between the {001} and {101} facets of anatase. As indicated in the slab model, two independent parameters b and a denote lengths of the side of the bipyramid and the side of the square {001} 'truncation' facets, respectively.

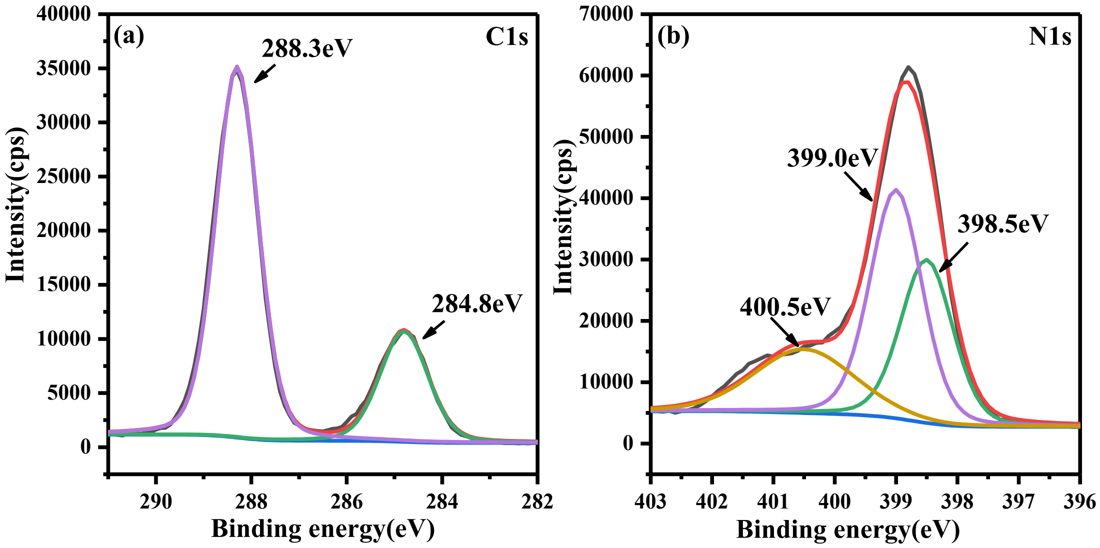

Figure S1. XPS spectra of pure g-C_3N_4: C 1s spectra (a) and N 1s spectra (b).

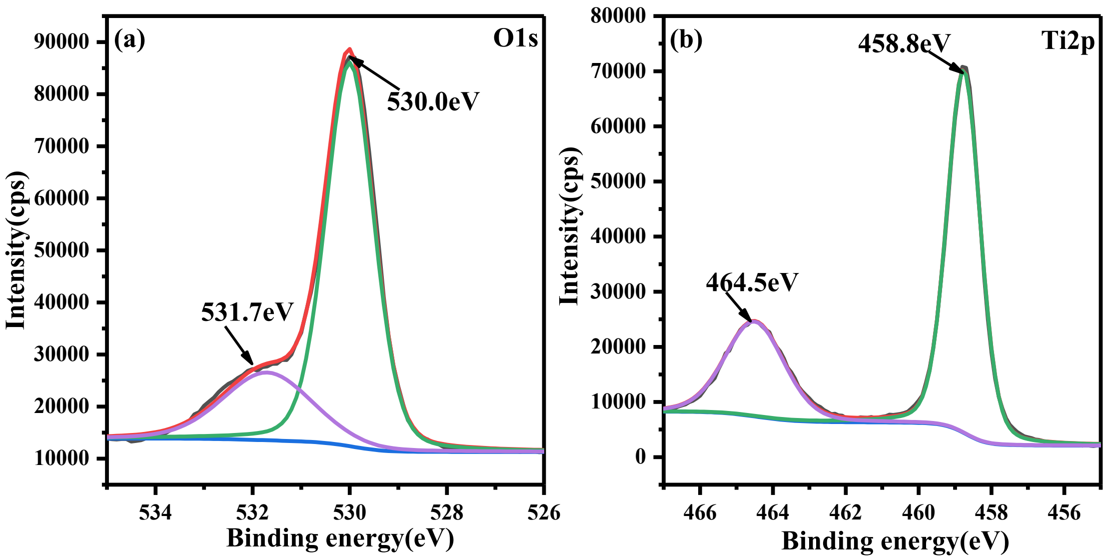

Figure S2. XPS spectra of pure (101)-(001)-TiO_2: O 1s spectra (a) and Ti 2p spectra (b).

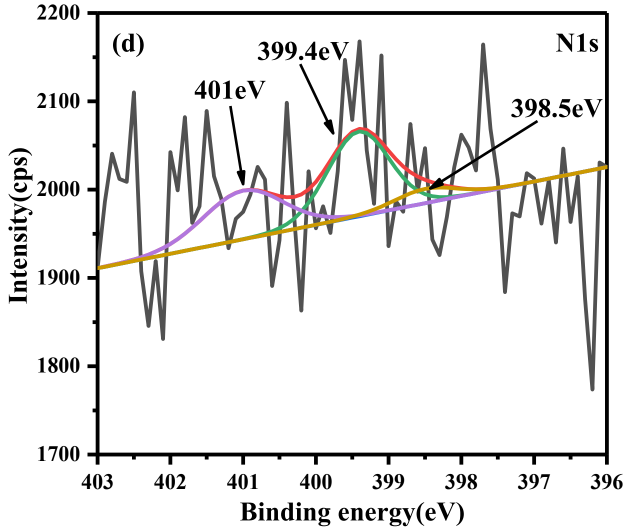

Figure S3. N 1s spectra of g-C_3N_4/(101)-(001)-TiO_2

Table S1. g-C_3N_4; g-C_3N_4/(101)-(001)-TiO_2 samples for details of C 1s peak fitting.

Sample	C 1s, g-C_3N_4			C 1s, g-C_3N_4/(101)-(001)-TiO_2		
Fitting conditions	Boundary: High BE=291.0 eV; Low BE=280.6 eV; Slope=0; $\sum x^2 = 18.89$			Boundary: High BE=290.2 eV; Low BE=282 eV; Slope=0; $\sum x^2 = 2.19$		
B.E. (eV)	284.8 eV C-C/C=C	/	288.3 eV N-C=N	284.7 eV C-C/C=C	286.2 eV C-OH	288.6 eV N-C=N

Table S2. g-C_3N_4;g-C_3N_4/(101)-(001)-TiO_2 samples for details of N 1s peak fitting.

Sample	N 1s, g-C_3N_4			N1s, g-C_3N_4/(101)-(001)-TiO_2		
Fitting conditions	Boundary: High BE=403 eV; Low BE=394 eV; Slope=0; $\sum x^2 = 9.12$			Boundary: High BE=403 eV; Low BE=394 eV; Slope=0; $\sum x^2 = 2.34$		
B.E. (eV)	398.5 eV C-N=C	399.0 eV N-C_3	400.5 eV NH_X	398.5 eV C-N=C	399.4 eV N-C_3	401.0 eV NH_X

Table S3. (101)-(001)-TiO_2; g-C_3N_4/(101)-(001)-TiO_2 samples for details of O 1s peak fitting.

Sample	O1s, (101)-(001)-TiO_2			O1s, g-C_3N_4/(101)-(001)-TiO_2		
Fitting conditions	Boundary: High BE=535 eV; Low BE=525.6 eV; Slope=0; $\sum x^2 = 10.14$			Boundary: High BE=535 eV; Low BE=525.7 eV; Slope=0; $\sum x^2 = 7.48$		
B.E. (eV)	530.0 eV (N)$_2$C-OH	531.7 eV H_2O	/	529.9 eV (N)$_2$C-OH	531.7 eV H_2O	/

Table S4. (101)-(001)-TiO_2; g-C_3N_4/(101)-(001)-TiO_2samples for details of Ti 2p peak fitting.

Sample	Ti 2p, g-C_3N_4		Ti 2p, g-C_3N_4/(101)-(001)-TiO_2	
Fitting conditions	Boundary: High BE=467 eV; Low BE=455 eV; Slope=0; $\sum x^2 = 8.20$		Boundary: High BE=467 eV; Low BE=455 eV; Slope=2; $\sum x^2 = 11.9$	
B.E. (eV)	458.8 eV Ti 2p3/2	464.5 eV Ti 2p1/2	458.7 eV Ti 2p3/2	464.4 eV Ti 2p1/2

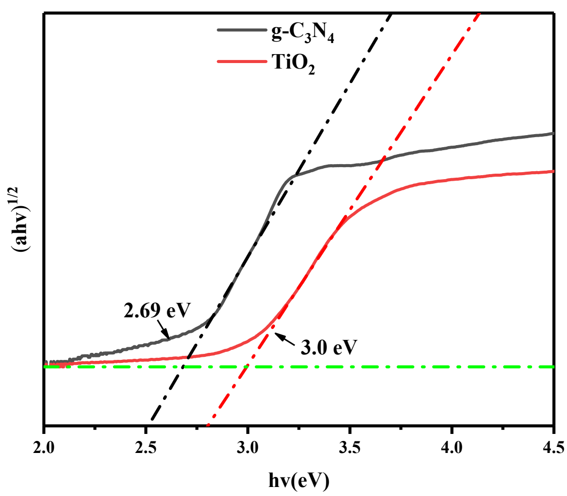

Figure S4. Band gap width diagram of g-C_3N_4 and (101)-(001)-TiO_2

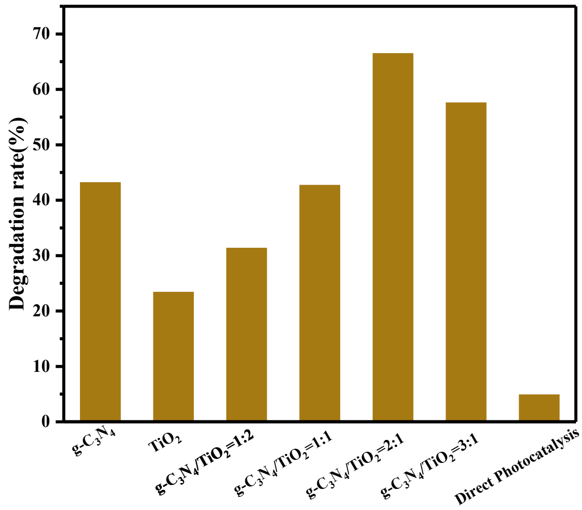

Figure S5. Paracetamol degradation rates of the as-prepared samples.

Table S5. Kinetic analysis of degradation of Paracetamol by the as-prepared samples.

Sample	The pseudo-first-order reaction kinetics	k（h^{-1}）	R^2
$g\text{-}C_3N_4$	ln（C_t/C_0）=-0.09272-0.08761x	0.1031	0.9191
TiO_2	ln（C_t/C_0）=0.02386-0.04614x	0.0422	0.9808
$g\text{-}C_3N_4/TiO_2$=1：2	ln（C_t/C_0）=0.02888-0.06592x	0.0611	0.9797
$g\text{-}C_3N_4/TiO_2$=1：1	ln（C_t/C_0）=0.00935-0.09405x	0.0923	0.9986
$g\text{-}C_3N_4/TiO_2$=2：1	ln（C_t/C_0）=0.00416-0.17534x	0.1746	0.9904
$g\text{-}C_3N_4/TiO_2$=3：1	ln（C_t/C_0）=0.01803-0.14096x	0.1379	0.9902
Direct photocatalysis	ln（C_t/C_0）=-0.0069-0.00861x	0.0098	0.8968

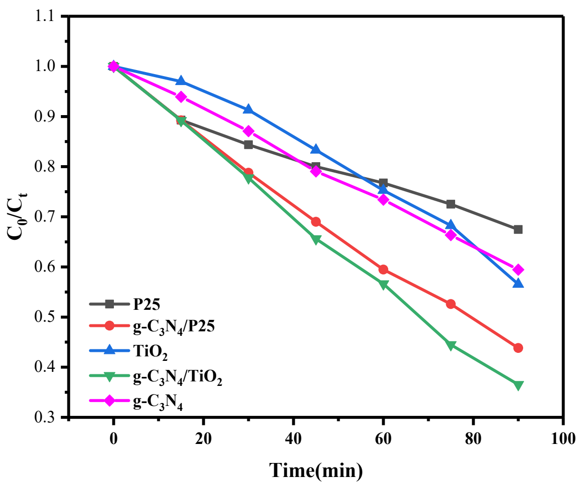

Figure S6. Photocatalytic degradation of MB by different photocatalysts under the irradiation of 300 W Xenon lamp (λ> 420 nm).

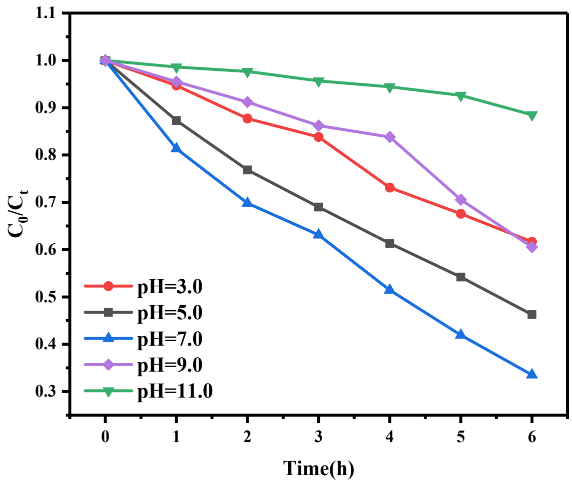

Figure S7. Effect of pH on photocatalytic activity of reaction system.

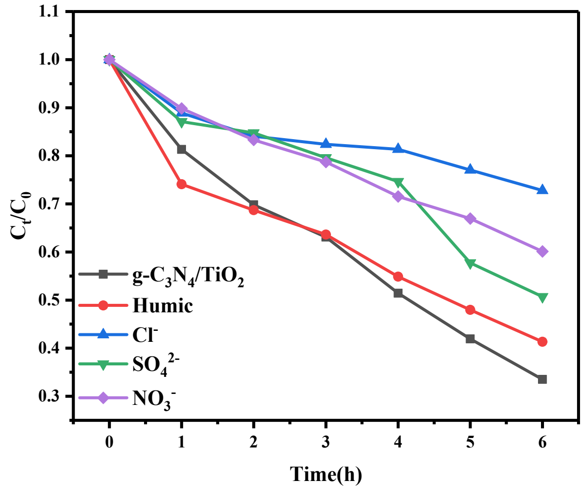

Figure S8. Effect of interfering ions on photocatalytic activity of reaction system.

Figure S9. ESR spectra of radical adducts ($\cdot O_2^-$ (a) and $\cdot$OH(a))trapped by DMPO in g-C_3N_4 and (101)-(001)-TiO_2 dispersion as a function of time under dark and visible light (in methanol dispersion for DMPO-$\cdot O_2^-$ and in aqueous for DMPO-$\cdot$OH).