

Supporting Information

Hydrogen-induced defective crystalline carbon nitride with enhanced bi-directional charge migration for persulfate photoactivation

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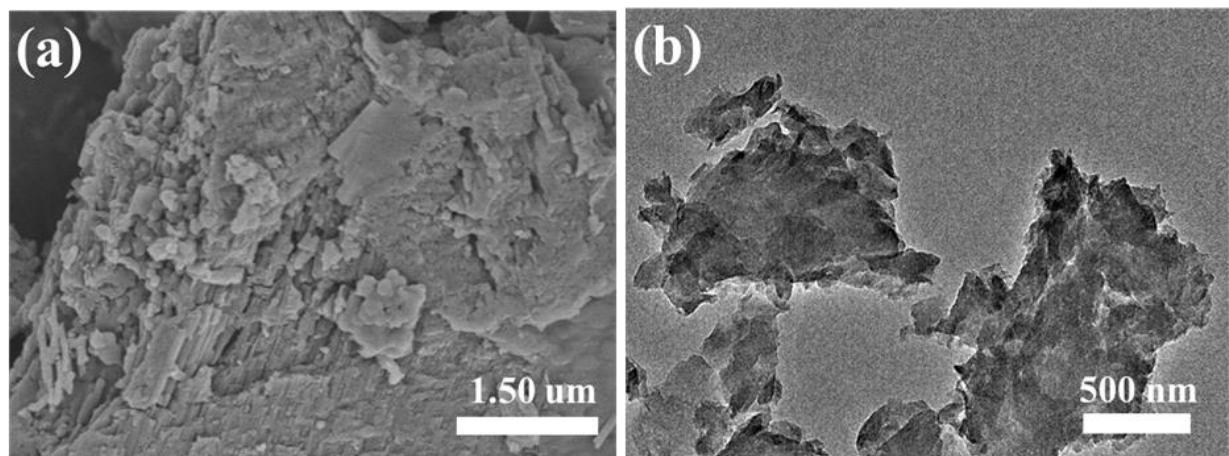


Figure S1. (a) SEM, (b) TEM image of g-C₃N₄.

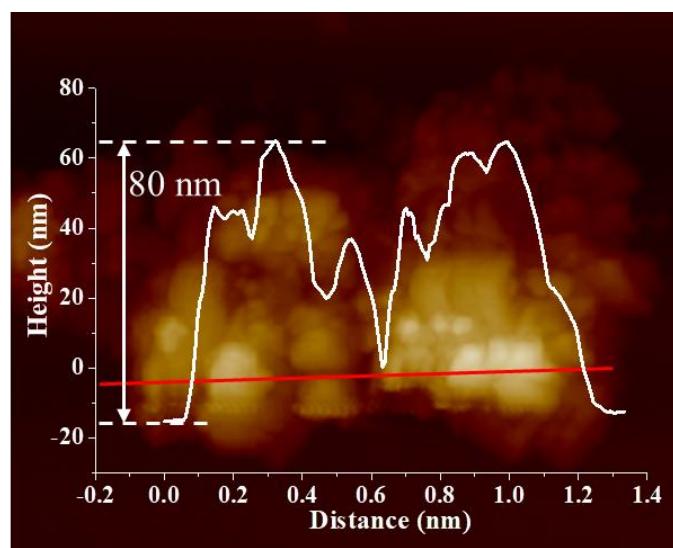


Figure S2. AFM image of g-C₃N₄.

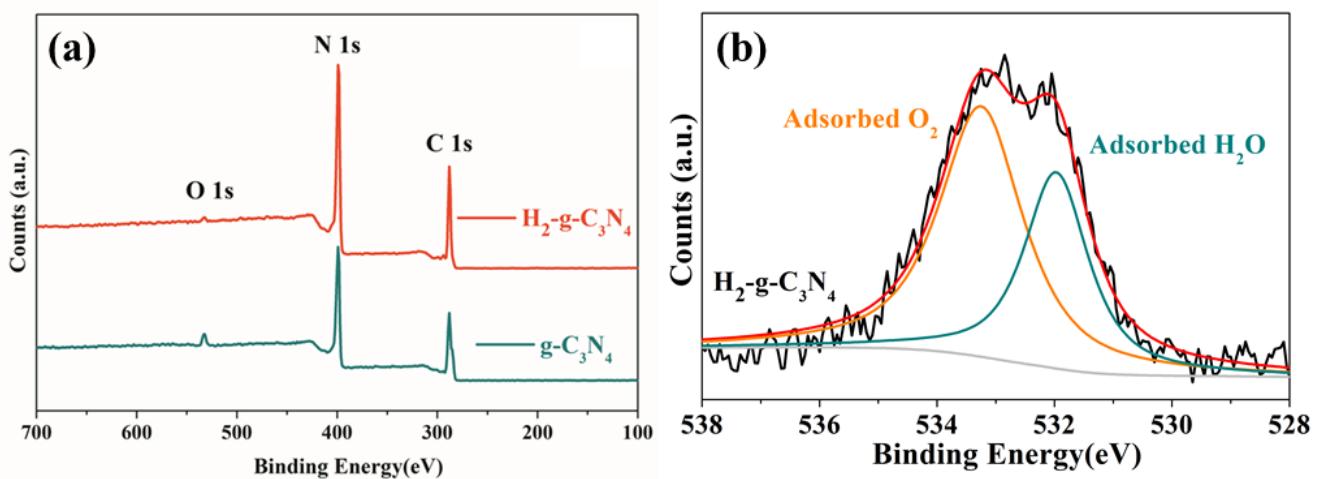


Figure S3. (a) XPS survey spectra for $\text{g-C}_3\text{N}_4$ and $\text{H}_2\text{-g-C}_3\text{N}_4$, (b) High resolution XPS spectrum of O1s in $\text{H}_2\text{-g-C}_3\text{N}_4$.

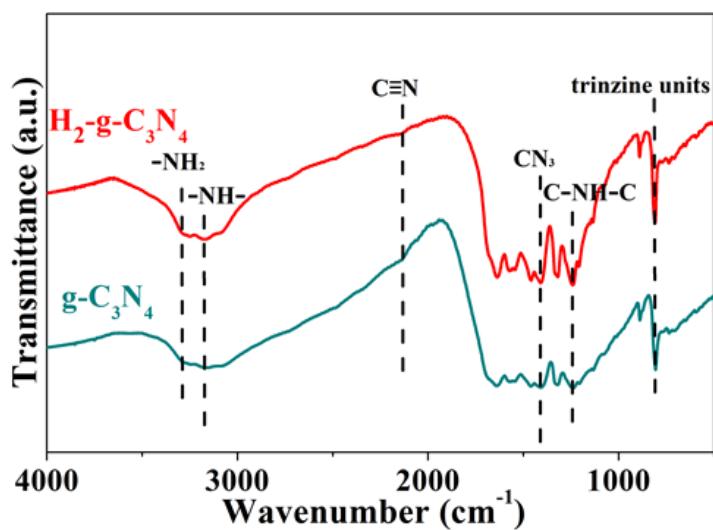


Figure S4. FTIR spectra of $\text{g-C}_3\text{N}_4$ and $\text{H}_2\text{-g-C}_3\text{N}_4$.

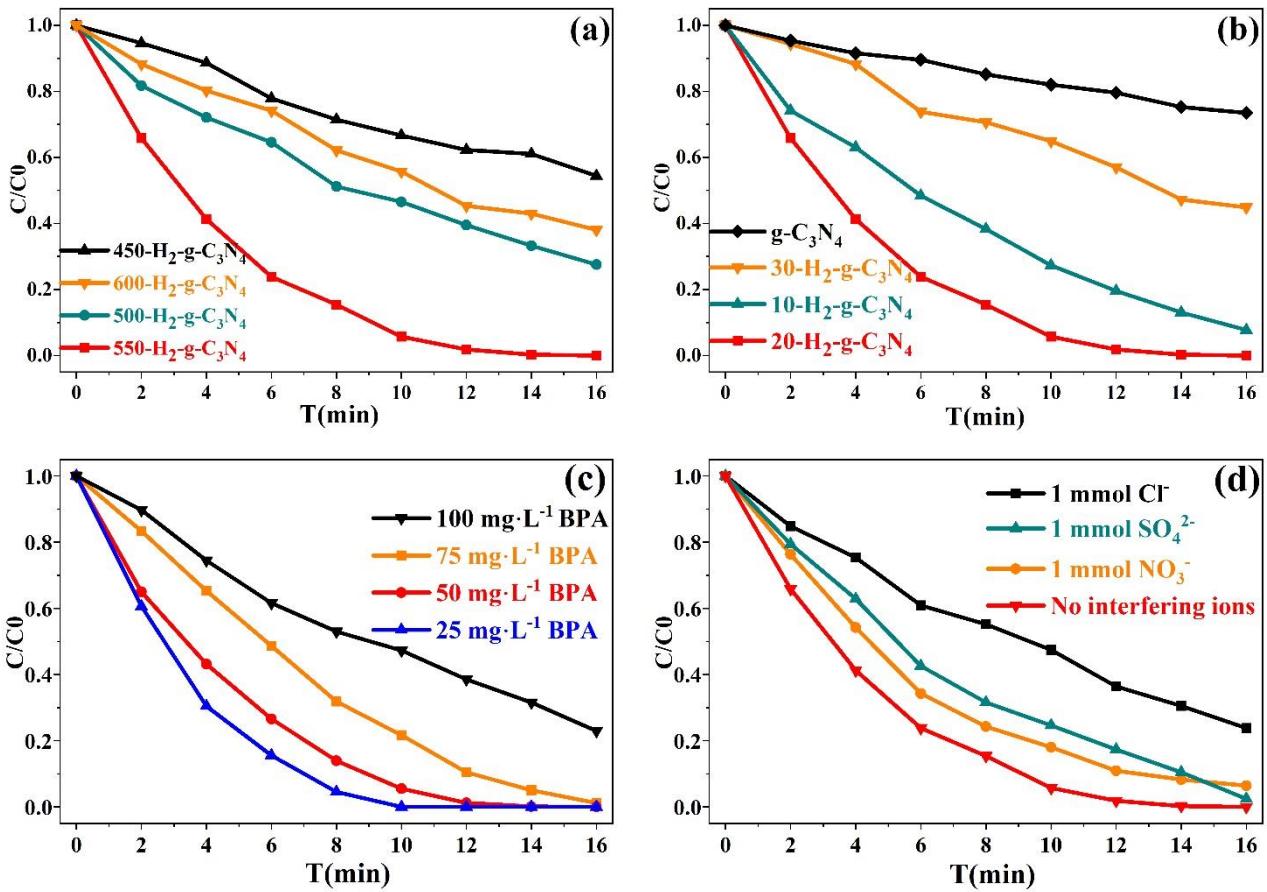


Figure S5. Effect of different calcination temperatures (a) and ventilation rate (b) on the efficiency of synergistic reactions. (c) The effect of BPA concentration and (d) inorganic anions on the synergistic degradation of BPA.

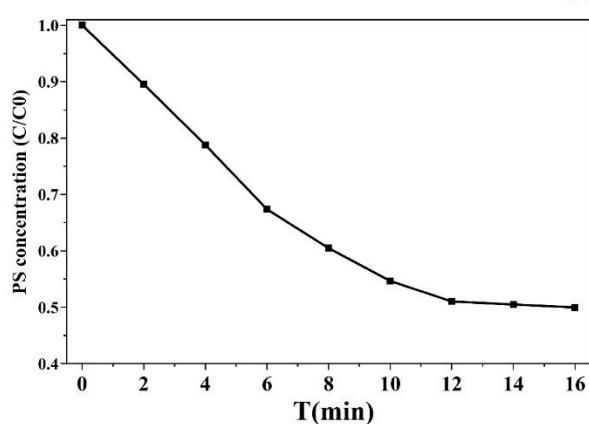


Figure S6. The change of persulfate concentration in the reaction solution as the reaction progresses.

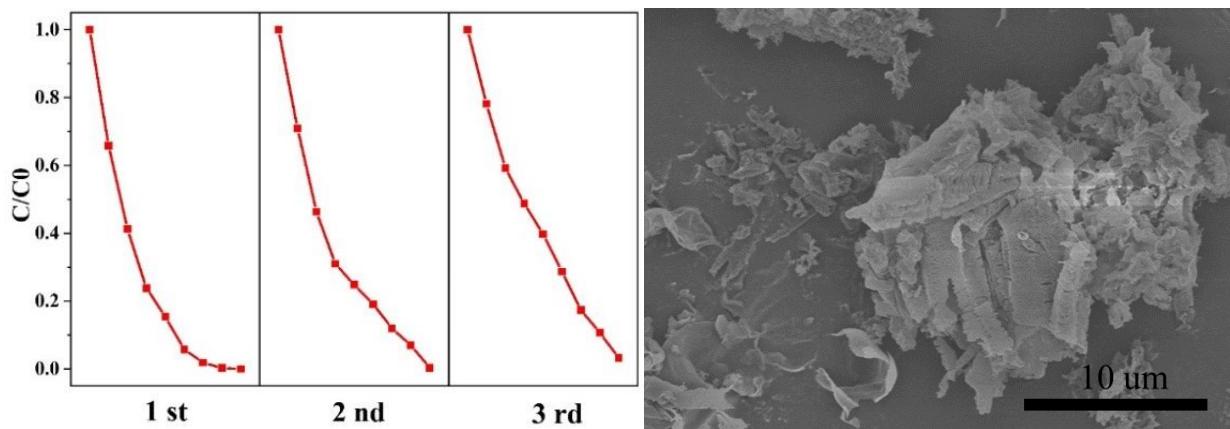


Figure S7. (a) Recycle tests of BPA degradation over H-g-C₃N₄ in the presence of persulfate and light irradiation. (b) SEM image of H-g-C₃N₄ after reactions.

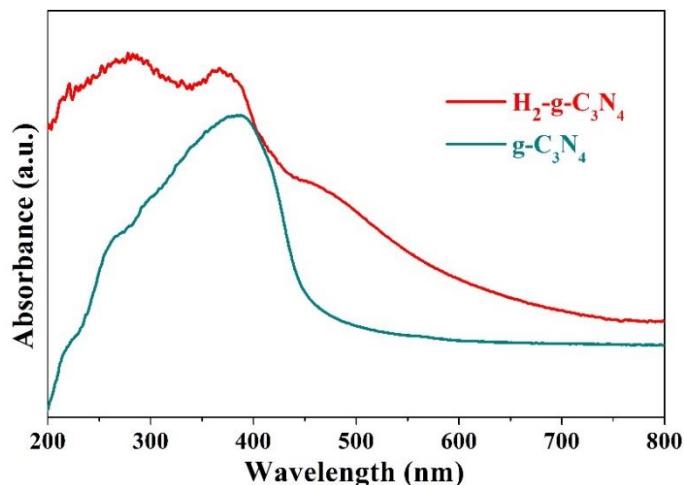


Figure S8. UV-vis diffuse reflectance spectra of g-C₃N₄ and H₂-g-C₃N₄.

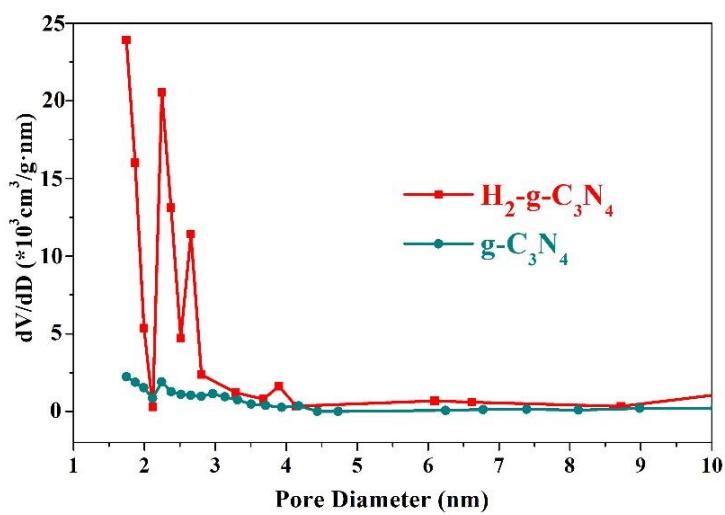


Figure S9. Pore size distribution curve of g-C₃N₄ and H₂-g-C₃N₄.

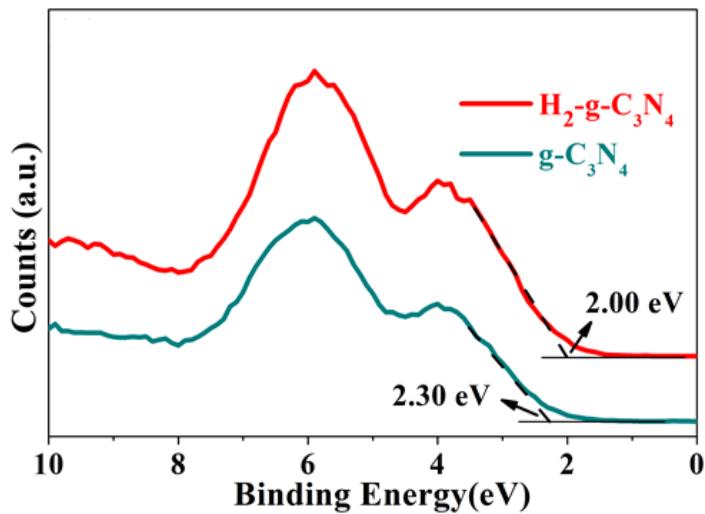


Figure S10. VB XPS spectra of $\text{g-C}_3\text{N}_4$ and $\text{H}_2\text{-g-C}_3\text{N}_4$.

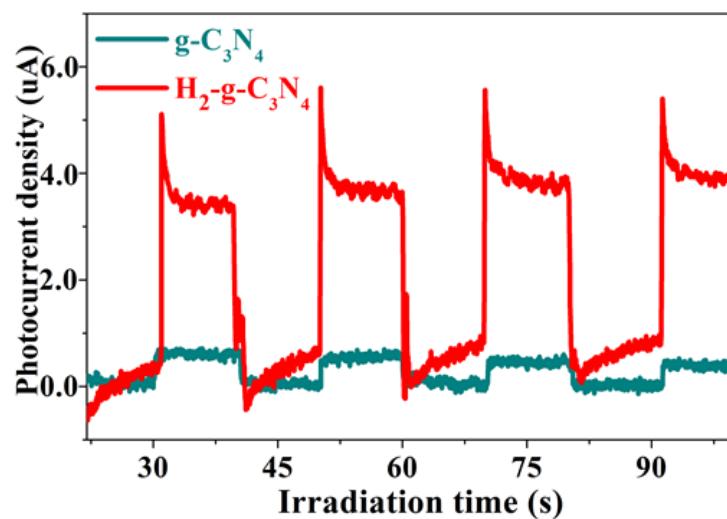


Figure S11. Photocurrent density curves of $\text{g-C}_3\text{N}_4$ and $\text{H}_2\text{-g-C}_3\text{N}_4$.

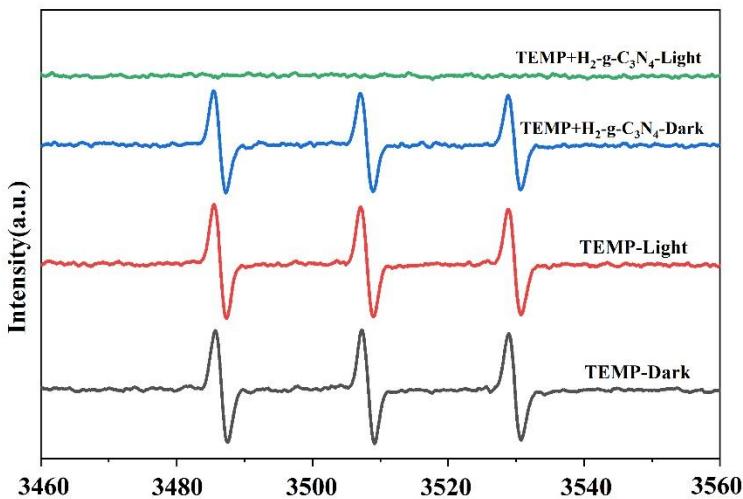


Figure S12. TEMP spin-trapping ESR spectra over $\text{H}_2\text{-g-C}_3\text{N}_4$ in different solvents.

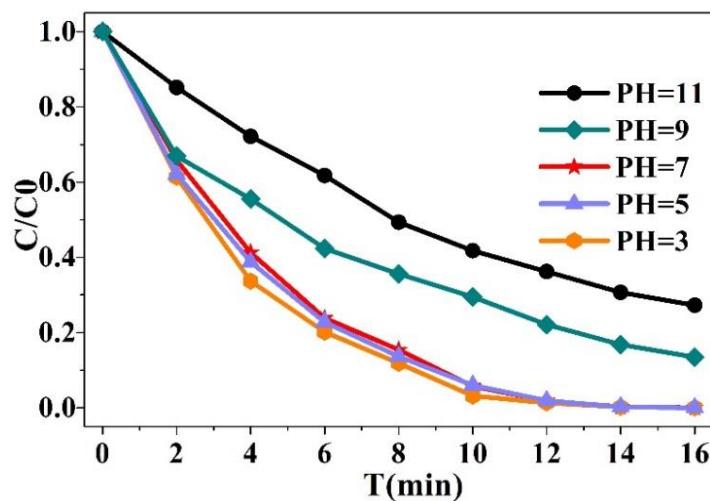


Figure S13. Degradation curves of BPA at different pH values over $\text{H}_2\text{-g-C}_3\text{N}_4$.

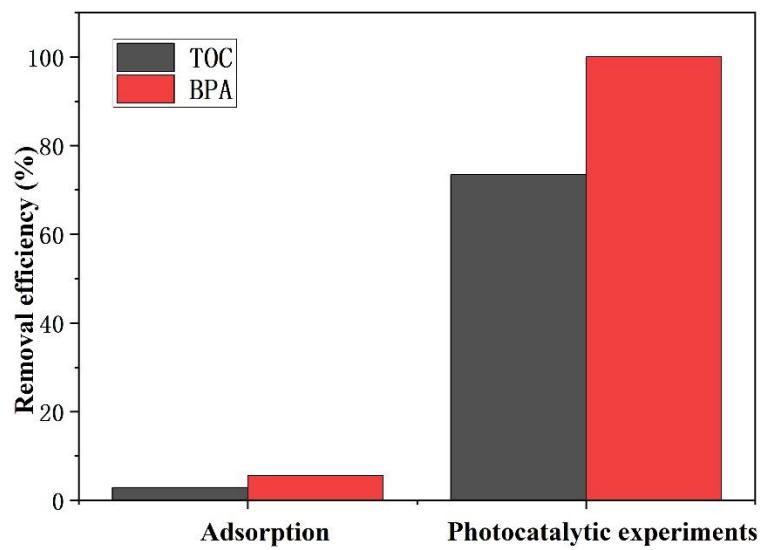


Figure S14. Pollutant removal efficiency by adsorption and photocatalytic.

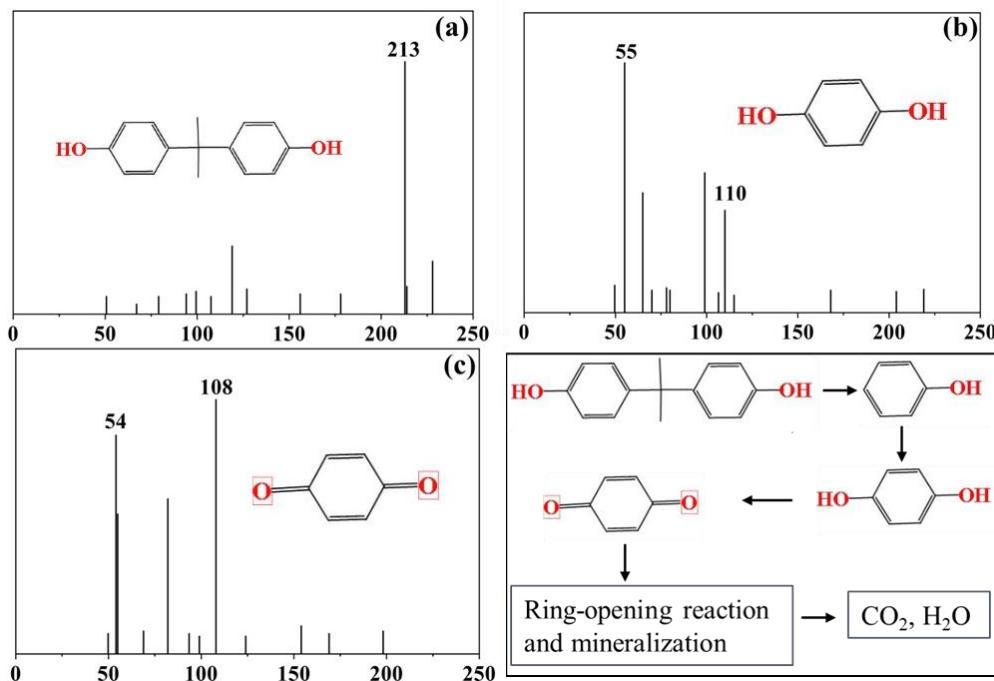


Figure S15. Proposed degradation pathway of BPA by $\text{H}_2\text{-g-C}_3\text{N}_4\text{+PS+Light}$ system.

Table S1. The binding energy of two atomic layer of $\text{g-C}_3\text{N}_4$ and $\text{H}_2\text{-g-C}_3\text{N}_4$.

	E_{1L}	E_{2L}	ΔE_{bind}
$\text{g-C}_3\text{N}_4$	-12394.89	-24795.31	-5.52
$\text{H}_2\text{-g-C}_3\text{N}_4$	-12120.85	-24248.82	-7.11

Table S2. XPS survey spectra of $\text{g-C}_3\text{N}_4$ and $\text{H}_2\text{-g-C}_3\text{N}_4$.

Sample	XPS			C/N ratio	N-H	N-(C)3	C-N=C
	(C) %	(N) %	(O) %				
$\text{g-C}_3\text{N}_4$	46.89	50.75	2.35	0.92	10.50	17.19	72.31
$\text{H}_2\text{-g-C}_3\text{N}_4$	49.48	43.01	6.75	1.15	22.35	30.42	47.23

Table S3. The comparison of performances of photocatalysts for BPA degradation efficiencies.

Catalyst	Light source	Catalyst Dosage (g/L)	PS/PMS Dosage (mM)	BPA Concentration (mg/L)	Complete Degradation time (time)	Rate constant (k, min ⁻¹)	Ref
BM200	300 W Xenon lamp	0.25	0.2	10	40	0.15	31
ECN60	300 W Xenon lamp ($\lambda > 420$ nm)	0.33	40.0	20	20	0.136	32
OVs-Zn ₂ SnO ₄	300W Xe-arc lamp ($\lambda > 420$ nm)	0.1	30.81	5	60	0.026	33
N,S:CQD/MIL-101(Fe)	350 W Xenon lamp ($\lambda > 400$ nm)	0.4	3.0	20	60	0.0551	34
g-C ₃ N ₄ /MIL-101(Fe)	300 W Xenon lamp ($\lambda > 400$ nm)	0.5	1.0	10	60	0.0589	35
Fe-POM/001-TiO ₂	300 W Xenon lamp 200 mw/cm ²	0.5	1.85	50	25	0.195	36
BiOI/Bi ₂ W _{0.25} Mo _{0.75} O ₆	300 W xenon lamp	1.0	1.5	15	30	0.06531	37
TGNF5@TOB C	300 W Xenon lamp ($\lambda > 420$ nm)	0.5	2.0	10	60	0.0522	38
CNBC	300 W Xenon lamp ($\lambda > 420$ nm)	1.0	1.0	5	60 (35%)	0.0559	39
Ag–Fe@BAB	250 W LED lamp ($\lambda = 400$ nm)	1.0	0.5	10	80	0.056	40
g-C ₃ N ₄ -NS	150 W Xenon lamp ($\lambda = 400$ nm)	0.5	5.0	5	60	0.0469	41
FeOOH@g-C ₃ N ₄	300 W Xenon lamp ($\lambda \geq 420$ nm)	0.4	2.0	20	60	0.0568	42
PDI-P9	800 W Xenon lamp ($\lambda > 420$ nm) low-pressure Hg	0.5	1.5	5	15	0.248	43
SCF@GCN	UV-Clamp ($\lambda = 240\text{--}260$ nm)	0.3	4.0	20	15	0.34	44
MIL-88B	visible light 200 mw/cm ²	0.6	2.0	10	25	0.107	45
H ₂ -g-C ₃ N ₄	300 W Xenon lamp 200 mw/cm ²	0.50	1.85	50	15	0.367	This Work

Table S4. BET surface areas and pore volumes of g-C₃N₄ and H₂-g-C₃N₄.

Sample	BET surface areas		pore volumes cm ³ .g ⁻¹
	m ² .g ⁻¹		
g-C ₃ N ₄	9.82		0.02
H ₂ -g-C ₃ N ₄	65.56		0.14

Table S5. Lifetime Components of g-C₃N₄ and H₂-g-C₃N₄.

material	τ_1 (ns)	τ_2 (ns)	τ_3 (ns)	τ_{ave} (ns)
C ₃ N ₄ (439nm)	1.87	6.207	45.37	9.48
H ₂ -g-C ₃ N ₄ (439nm)	6.73	31.25	1.69	8.99