

Supplementary Materials

Fe Single Atoms Reduced by NaBH_4 Mediate $\text{g-C}_3\text{N}_4$ Electron Transfer and Effectively Remove 2-Mercaptobenzothiazole

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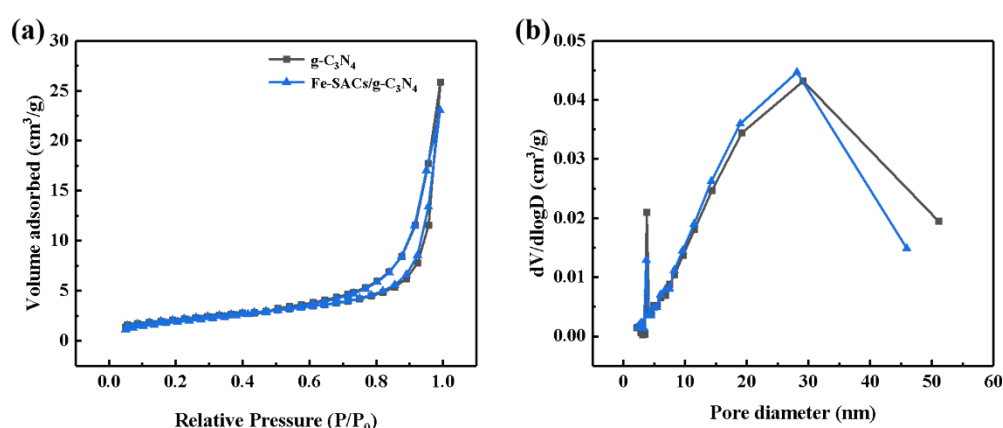


Figure S1. N_2 adsorption-desorption isotherms of the $\text{g-C}_3\text{N}_4$ and $\text{Fe-SACs/g-C}_3\text{N}_4$ (a) BJH pore size distribution curves of as-prepared photocatalysts (b).

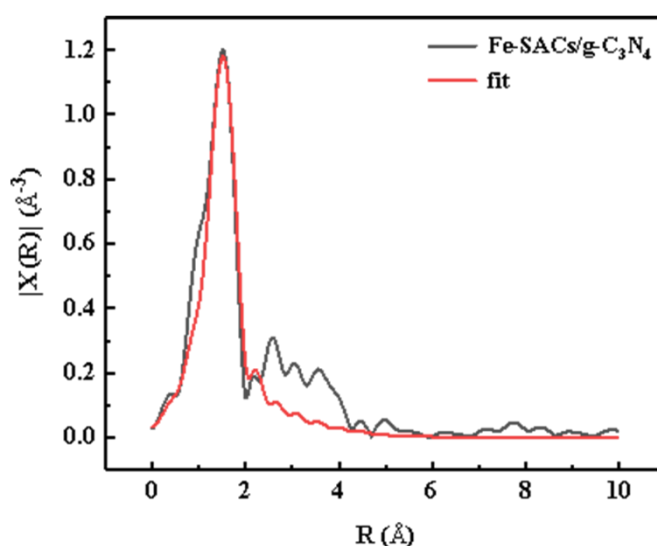


Figure S2. The EXAFS R space fitting curves of $\text{Fe-SACs/g-C}_3\text{N}_4$.

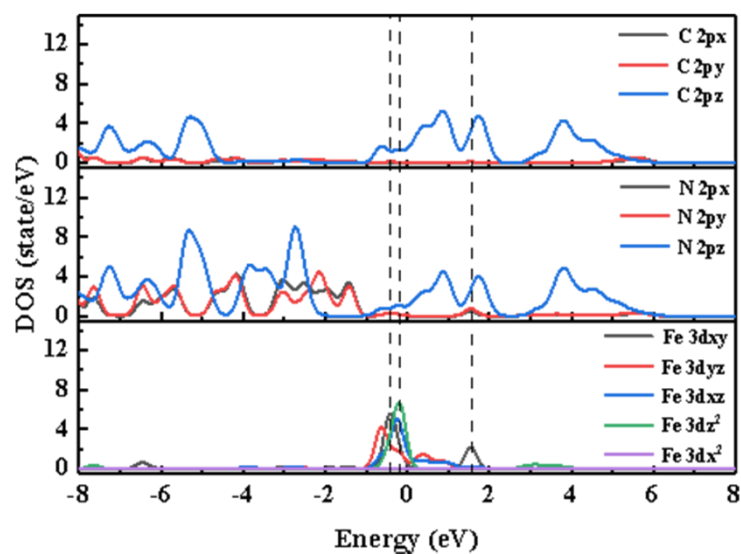


Figure S3. Projected density of states of the Fe-N4 system.

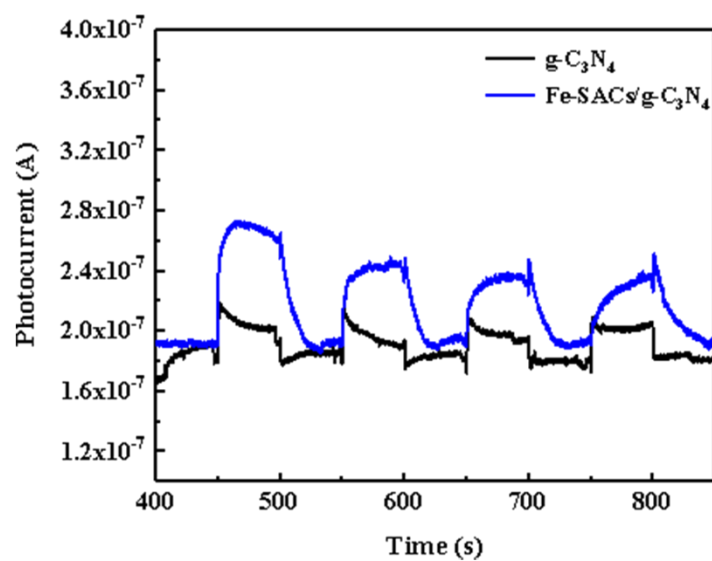


Figure S4. Photocurrent density of the g-C₃N₄ and Fe-SACs/g-C₃N₄.

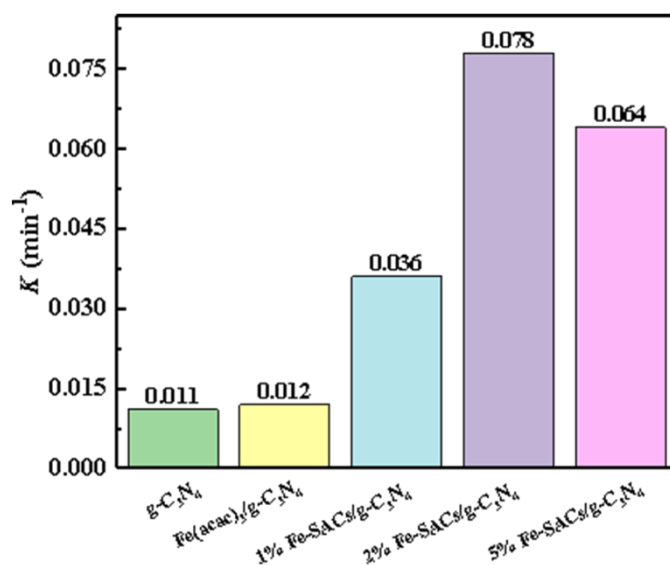


Figure S5. Degradation rate constants of different photocatalysts.

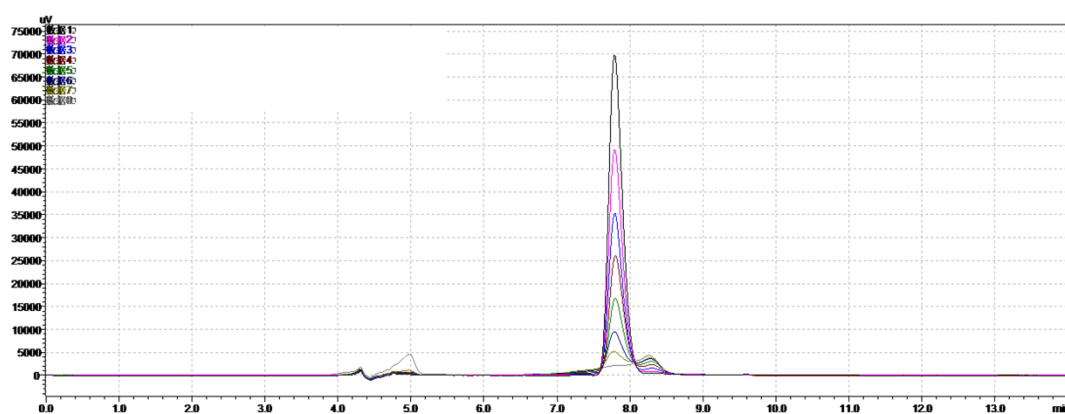


Figure S6. UV-Vis spectral changes of MBT during photoreaction.

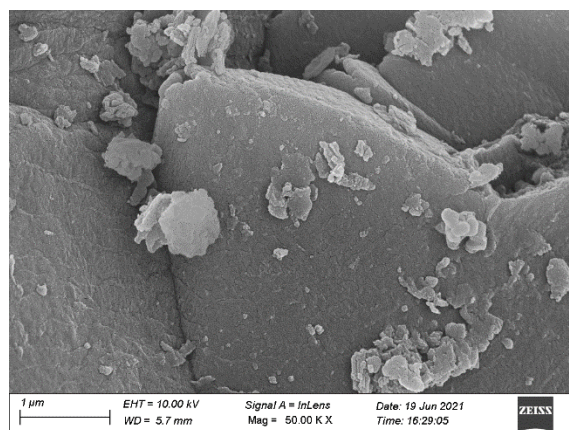


Figure S7. SEM of used Fe-SACs/ $\text{g-C}_3\text{N}_4$ photocatalyst.

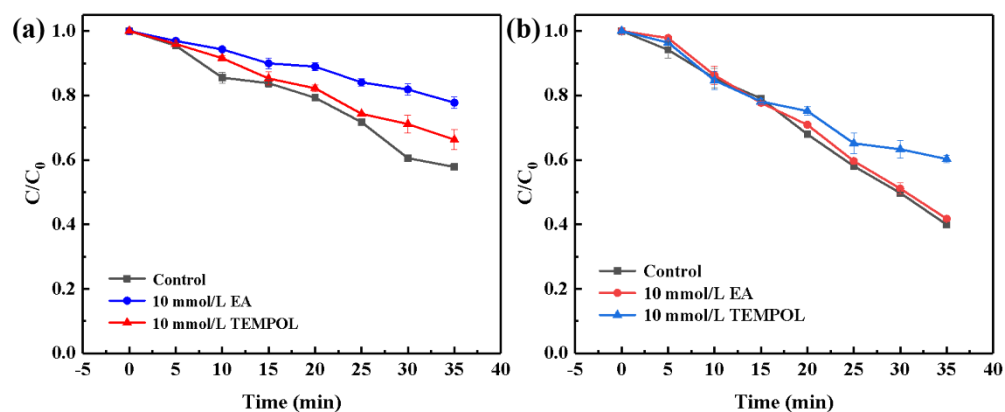


Figure S8. The photocatalytic activity of $g-C_3N_4$ (a), $Fe(acac)_3/g-C_3N_4$ (b) for degrading MBT with the presence of various scavengers.

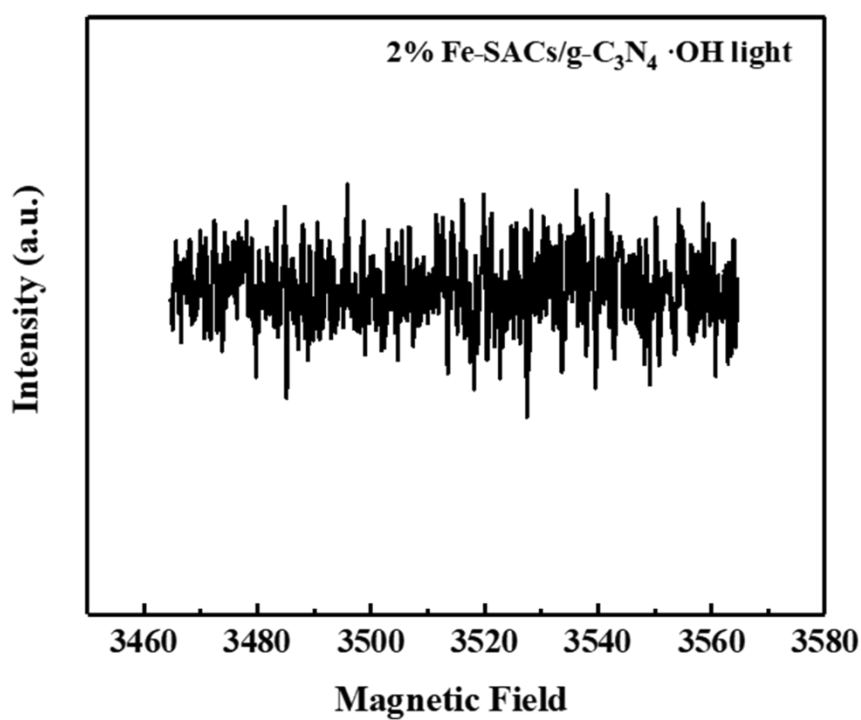


Figure S9. The EPR spectrum of DMPO-OH in the presence of Fe-SACs/g-C₃N₄.

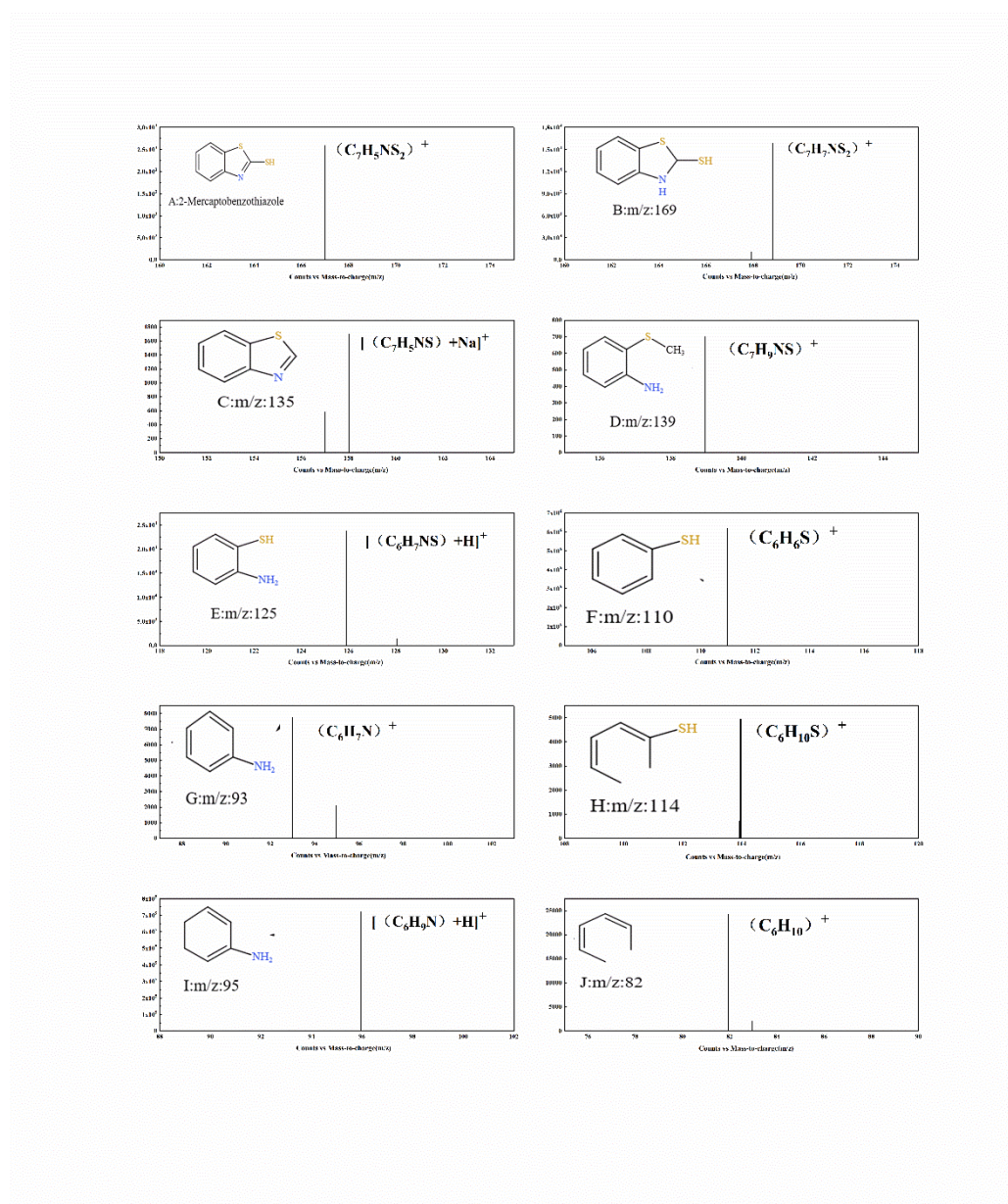


Figure S10. LC-MS spectra of MBT intermediates in the degradation reaction with Fe-SACs/g-C₃N₄.

Table S1. ICP Test Details.

Sample	Sampling Quality/g	Constant Volume/mL	Measured Element	Instrument Readings	Quality Score %
2% Fe-SACs/g-C ₃ N ₄	0.0141	25	Fe	0.59228	0.1050%

Table S2. The FWHM data and crystallite size of (002) peak.

	g-C ₃ N ₄	Fe(acac) ₃ /g-C ₃ N ₄	Fe-SACs/g-C ₃ N ₄
FWHM	2.22	2.23	2.43
crystallite size	3.85	3.82	3.51

Table S3. Parameters of EXAFS fits for Fe-SACs/g-C₃N₄.

Sample	Shell	N ^a	R (Å) ^b	σ^2 (Å ² ·10 ⁻³) ^c	ΔE_0 (eV) ^d	R factor (%)
Fe foil	Fe-Fe1	8*	2.473-/±0.016	5.32-/±0.64	3.54-/±1.89	0.7
	Fe-Fe2	6*	2.813-/±0.023	6.45-/±1.81	5.23-/±2.10	
Sample	Fe-N	4.2-/±0.3	2.010-/±0.026	5.79-/±3.90	0.73/±4.70	1.4%

^a N: coordination numbers; ^b R: bond distance; ^c σ^2 : Debye-Waller factors; ^d ΔE_0 : the inner potential correction. R factor: goodness of fit.