

# Supplementary Material

## **Enhanced Photocatalytic Hydrogen Peroxide Production over g-C<sub>3</sub>N<sub>4</sub>/MoS<sub>2</sub> composites through Phase-Interface Engineering: Electron Transfer and Synergy Mechanism**

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## Figures

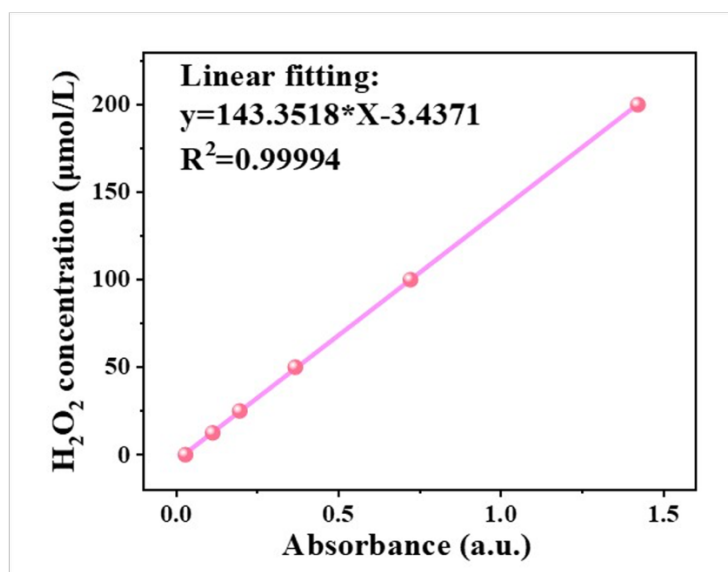


Fig. S1 Linear fitting equation of H<sub>2</sub>O<sub>2</sub> concentration determined by iodimetry.

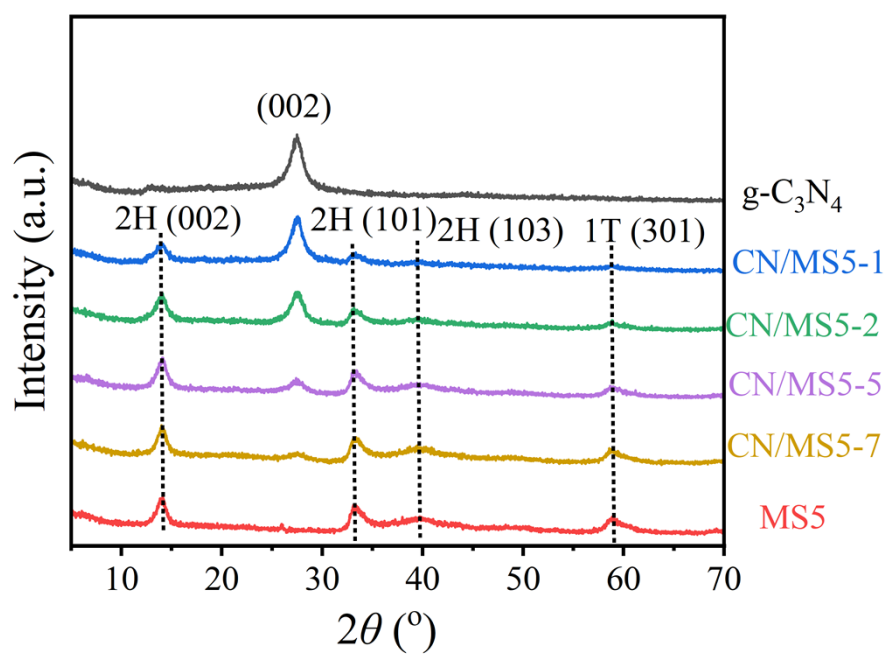
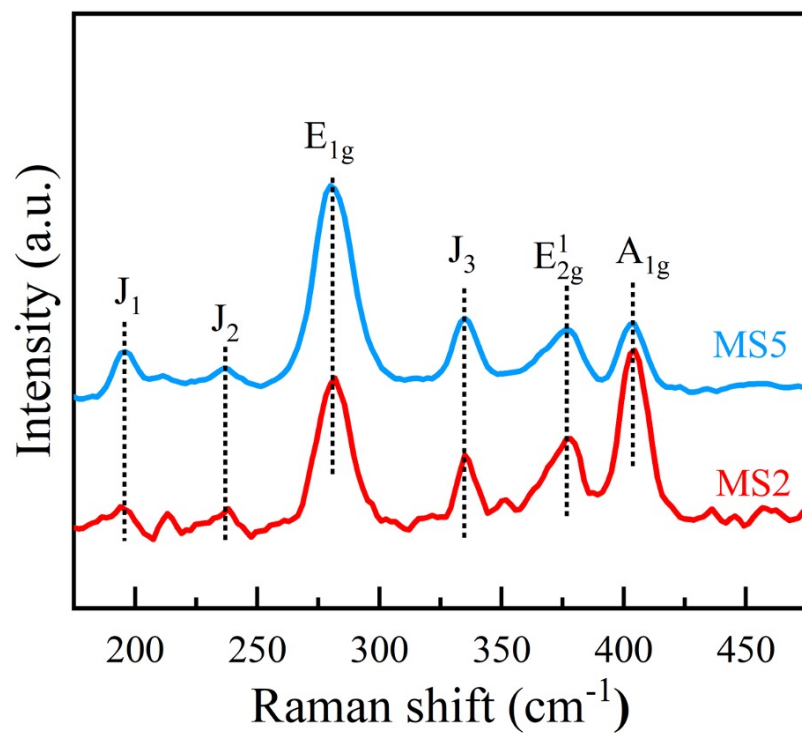
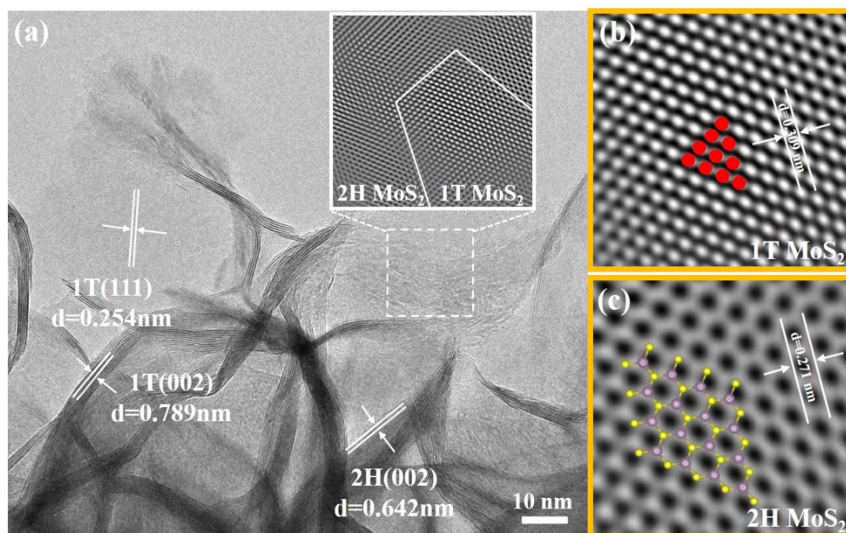


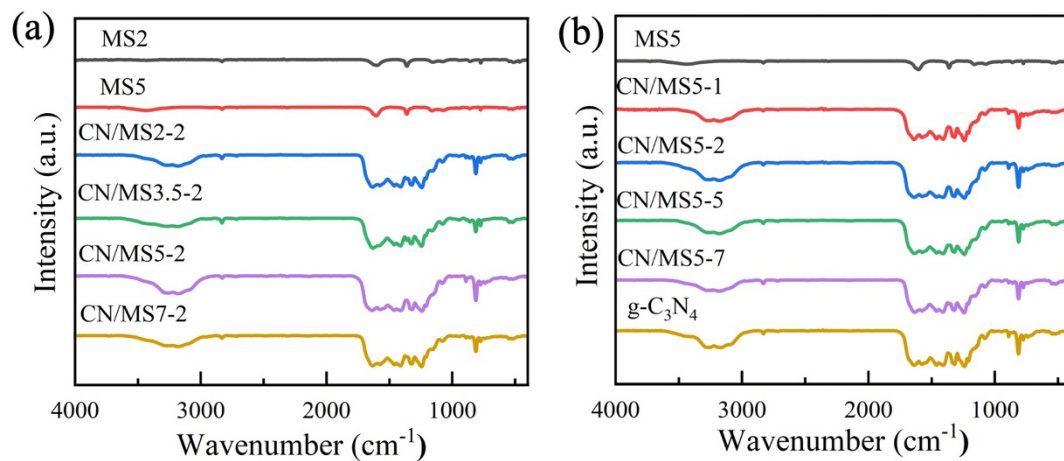
Fig. S2 XRD patterns of the CN/MS5-based heterojunctions



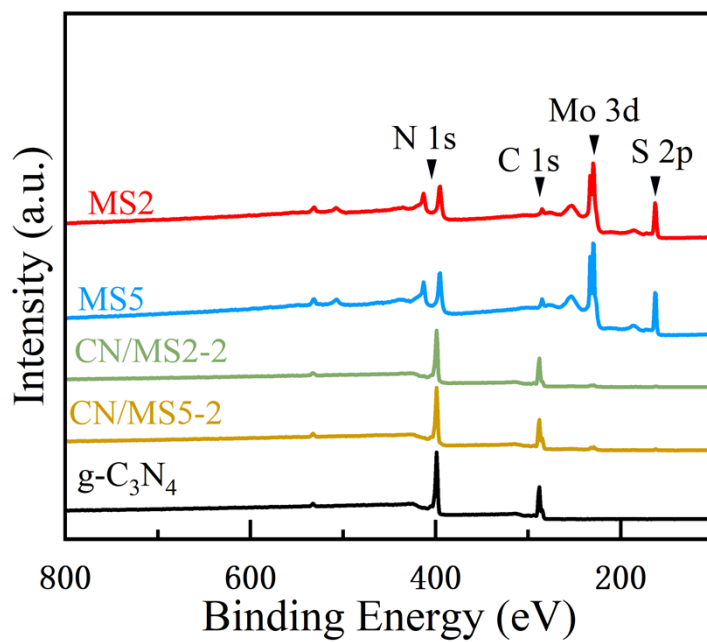
**Fig. S3** Raman spectra of MS2 and MS5



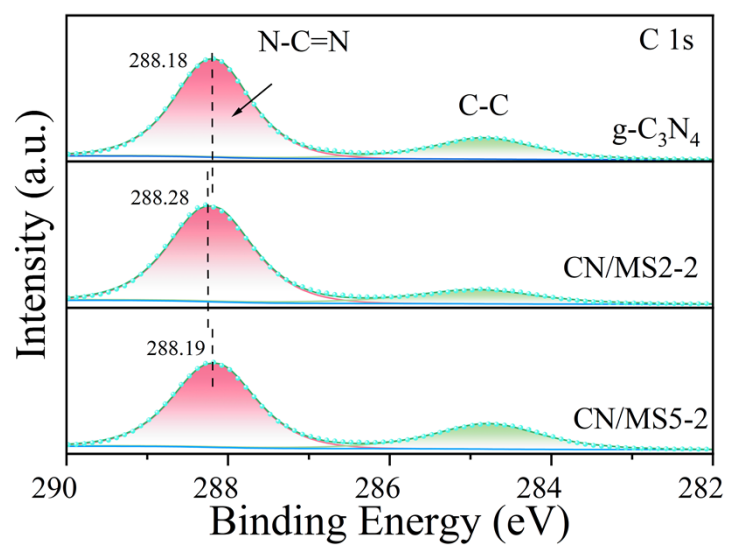
**Fig. S4** (a) TEM image of MS2. HRTEM images for (b) 1T-phase MoS<sub>2</sub> and (c) 2H-phase MoS<sub>2</sub>, respectively.



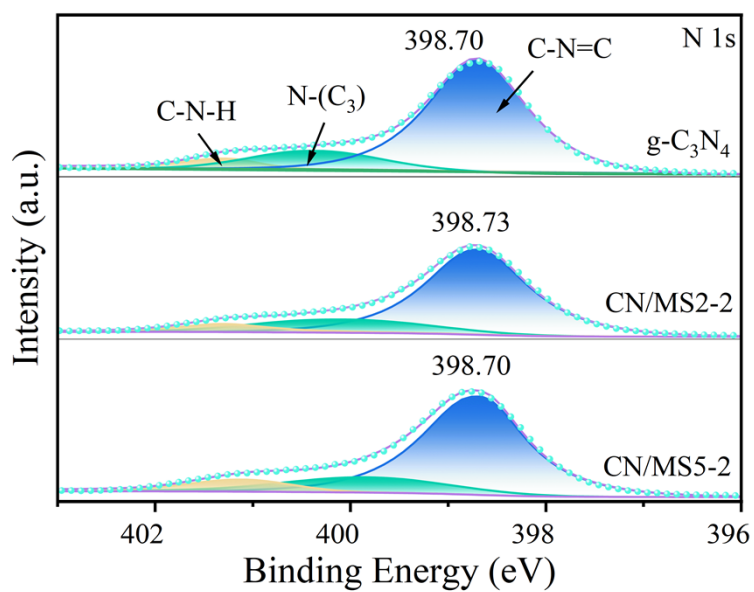
**Fig. S5** FT-IR spectra of various samples.



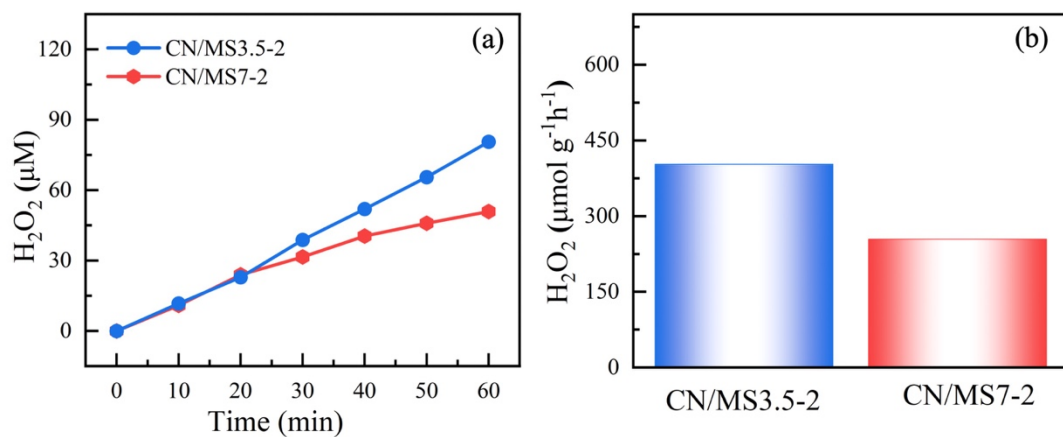
**Fig. S6** XPS spectra of g-C<sub>3</sub>N<sub>4</sub>, MS2, MS5, CN/MS2-2, and CN/MS5-2.



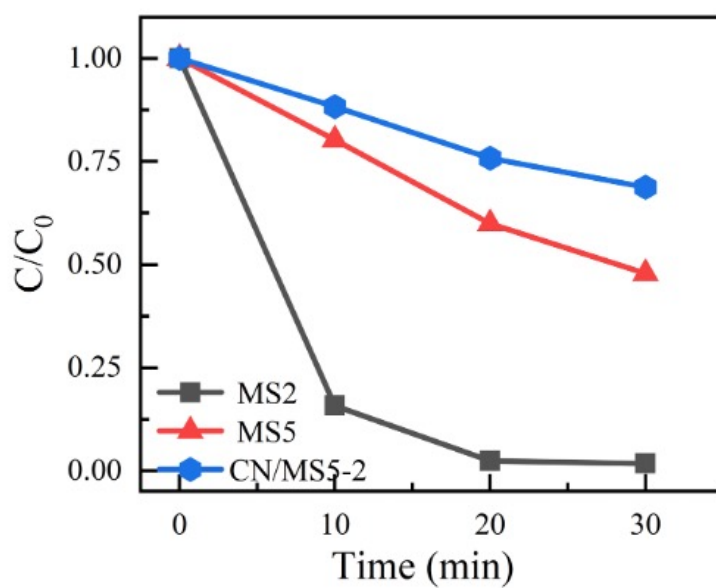
**Fig. S7** High-resolution XPS spectra of C 1s



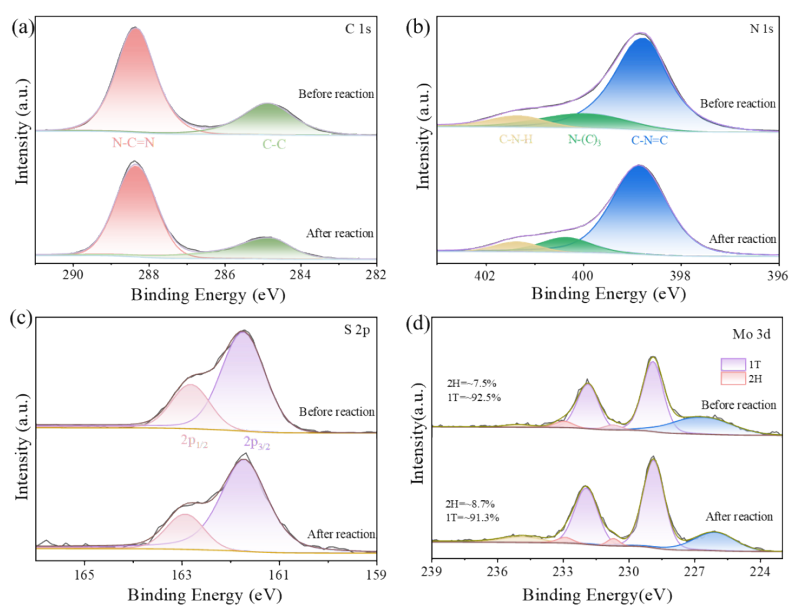
**Fig. S8** High-resolution XPS spectra of N 1s



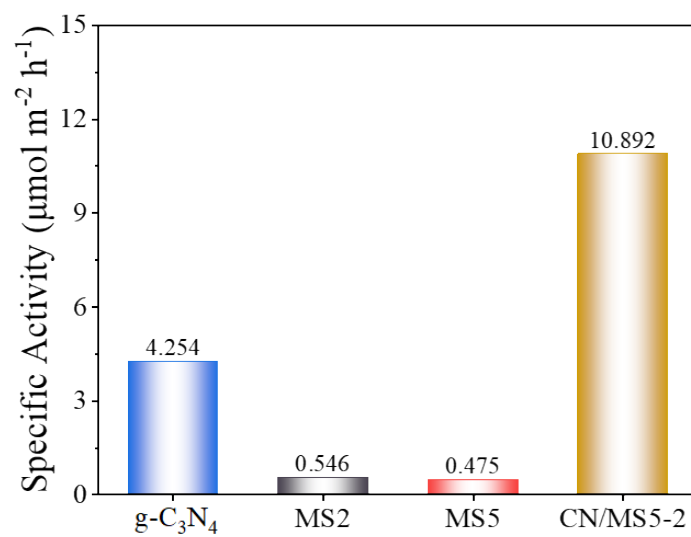
**Fig. S9** Photocatalytic  $\text{H}_2\text{O}_2$  production and corresponding yield on CN/MS3.5-2 and CN/MS7-2 catalysts.



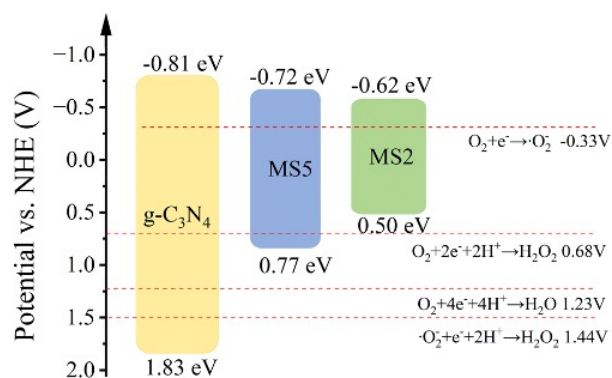
**Fig. S10** Decomposition of  $\text{H}_2\text{O}_2$  by MS2, MS5, and CN/MS5-2 under  $\text{N}_2$  conditions



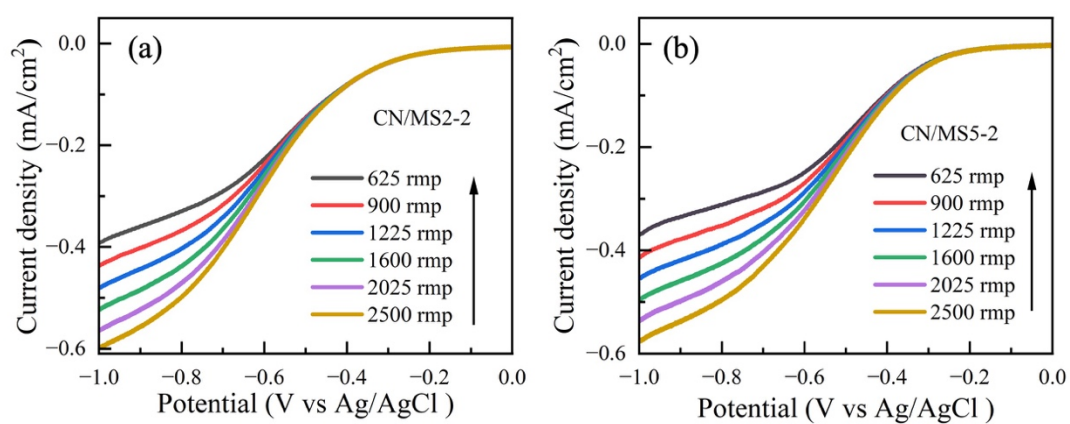
**Fig. S11** High-resolution XPS spectra of (a) C 1s, (b) N 1s, (c) 2p, and (d) Mo 3d for CN/MS5-2 before and after photocatalytic reaction.



**Fig. S12** Unit area activity of the sample



**Fig. S13** Energy band structures for g-C<sub>3</sub>N<sub>4</sub>, MS2, and MS5.



**Fig. S14** LSV curves of (a) CN/MS2-2 and (b) CN/MS5-2.