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WS_2/g-C_3N_4 Composite as an Efficient Heterojunction Photocatalyst for Biocatalyzed Artificial Photosynthesis

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1. Synthesis process of various composite samples

1.1 Synthesis of sample 1:

100 mg of g-C_3N_4 and 5 mg of WS_2 were added in 100 mL of water and then ultrasonically dispersed for 1.5 hours, and finally evaporated the solvent, sample 1 were obtained.

1.2 Synthesis of sample 2:

100 mg of g-C_3N_4 and 5 mg of WS_2 were added in 100 mL of water, and then the mixture was sealed into a 100 mL Teflon-lined stainless steel autoclave and heated to 140 ºC for 6 h. After cooling down to room temperature then evaporating the solvent, sample 2 were obtained.

1.3 Synthesis of sample 3:

100 mg of g-C_3N_4 and 5 mg of WS_2 were added in 100 mL of water, and then ultrasonically dispersed for 1.5 hours, then the dispersion was sealed into a 100 mL Teflon-lined stainless steel autoclave and heated to 140 ºC for 6 h. After cooling down to room temperature then evaporating the solvent, sample 3 were obtained.

1.4 Synthesis of sample 4:

The synthesis method is the same as sample 1.3, the only difference being that the hydrothermal time is changed to 2 hours.

1.5 Synthesis of sample 5:

The synthesis method is the same as sample 1.3, the only difference being that the hydrothermal temperature is changed to 120ºC.

2. Detection of reactive species

The procedures of the scavenging experiments of reactive oxygen species were similar to that of the photodegradation experiment. Various scavengers were subjected into the RhB solution prior to addition of photocatalyst, and the concentration of scavengers was the same at 1 mM. In this study, isopropyl alcohol (IPA), triethanolamine (TEOA) and nitrogen are used as scavengers of the hydroxyl radical, hole, and the superoxide radical, respectively; and KI acts as a scavenger of both hydroxyl radicals and holes.

3. Additional characterization

Raman measurement was carried out on a LabRAM HR800 Raman system using an excitation source of 532 nm laser.

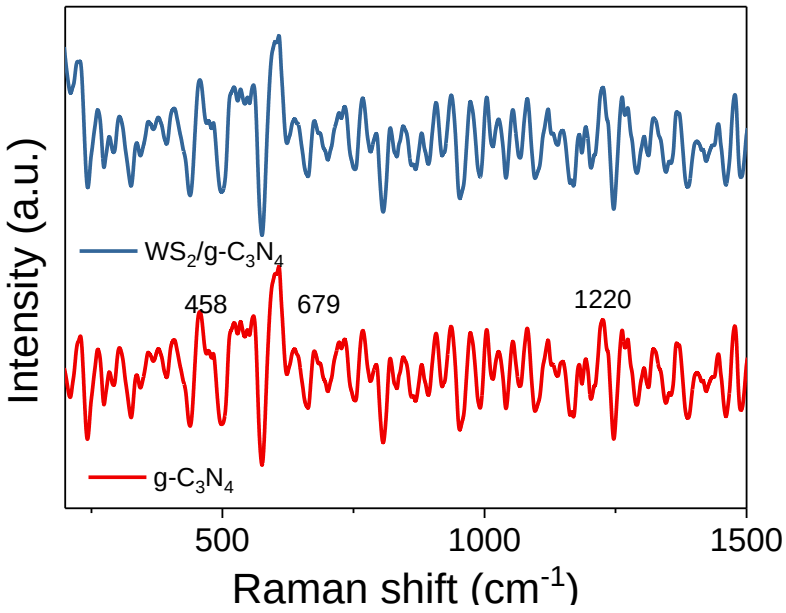

Figure S1. Raman spectra of g-C_3N_4 and 5 wt% WS_2/g-C_3N_4 composite.

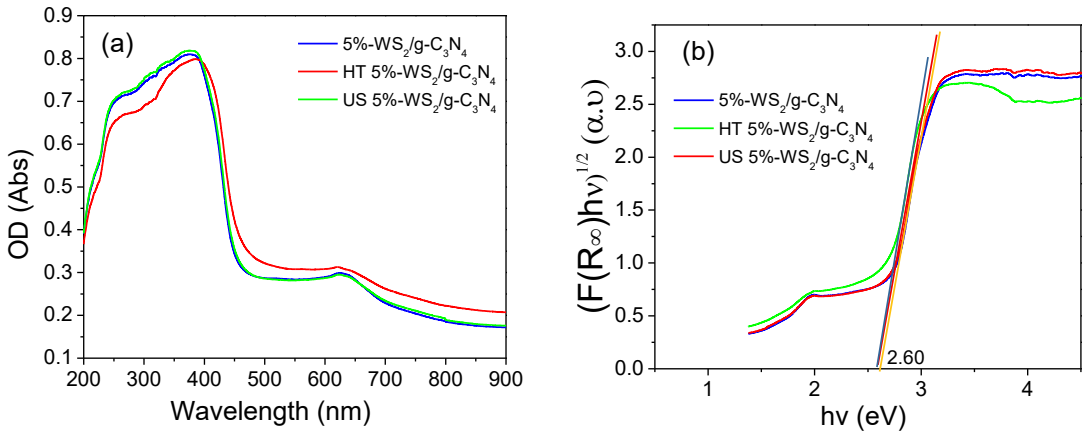

Figure S2. UV-vis absorption spectra (a) in the diffuse reflectance spectra mode of the composite with different preparation methods and (b) the corresponding bandgap estimated from Kubelka-Munk equation.

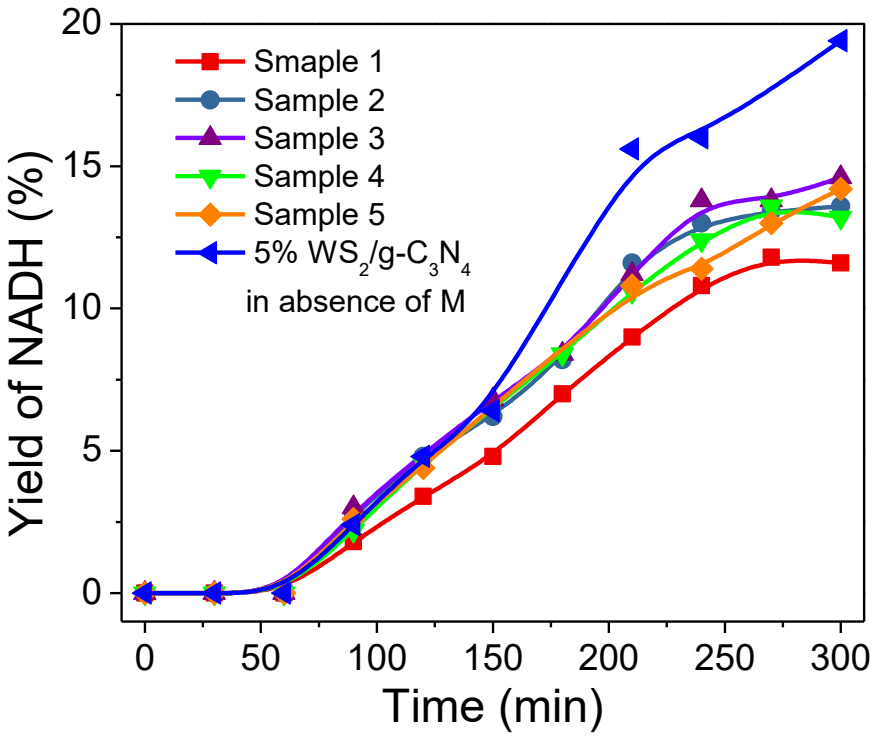

Figure S3. Photocatalytic NADH regeneration catalyzed by different composites samples. Detailed preparation conditions for each sample was summarized in Table S3.

Table S1. peak data of XPS spectra of g-C_3N_4, WS_2 and 5 wt% WS_2/g-C_3N_4 composite.

Catalyst	C 1s(eV)	N 1s(eV)	S 2p(eV)	W4f(eV)
g-C_3N_4	284.4, 288.0	398.4, 399.0, 400.5, 404.4	-	-
WS_2	-	-	162.9, 164.1	33.3, 35.5, 38.9
WS_2/g-C_3N_4	284.7, 288.2	398.7, 399.5, 401.0, 404.7	161.7, 163.0	32.1, 34.4, 37.6

Table S2. BET surface area, pore diameter and pore volume data of g-C_3N_4, 5 wt% WS_2/g-C_3N_4 composite and PM-WS_2/C_3N_4.

Sample	BET Surface Area(m^2/g)	Pore Diameter(nm)	Pore Volume(cm^3/g)
g-C_3N_4	7.34	28.15	0.05
5%-WS_2/g-C_3N_4	12.22	19.70	0.06
PM-WS_2/C_3N_4	6.87	23.50	0.04

Table S3. Photocatalytic NADH regeneration by composites with different treated methods.

Composite	Synthetic Methods	Yield of NADH at 6 h
Sample 1	Ultrasonication (1.5 h) without hydrothermal treatment	11.6%
Sample 2	Hydrothermal treatment (140ºC, 6 h) without ultrasonication	13.6%
Sample 3	Ultrasonication (1.5 h) + Hydrothermal treatment (140ºC, 6 h)	14.6%
Sample 4	Ultrasonication (1.5 h) + Hydrothermal treatment (140ºC, 2 h)	13.2%
Sample 5	Ultrasonication (1.5 h) + Hydrothermal treatment (120ºC, 6 h)	14.2%
5%-WS_2/g-C_3N_4	Ultrasonication (1.5 h) + Mechanical stirring (36 h) + Hydrothermal treatment (140ºC, 6 h)	37.1%
5%-WS_2/g-C_3N_4	Ultrasonication (1.5 h) + Mechanical stirring (36 h) + Hydrothermal treatment (140ºC, 6 h), photoregeneration of NADH in absence of M	19.4%