Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

S-scheme α-Fe_2O_3/g-C_3N_4 heterojunction nanostructure with superior visible-light photocatalytic activity for Aza-Henry reaction

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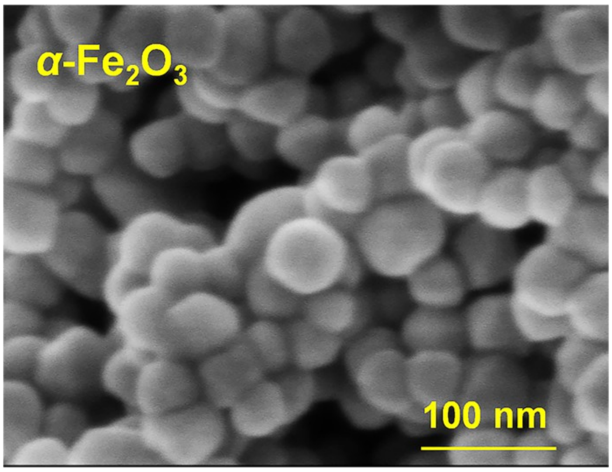

Figure S1. SEM image of α-Fe_2O_3.

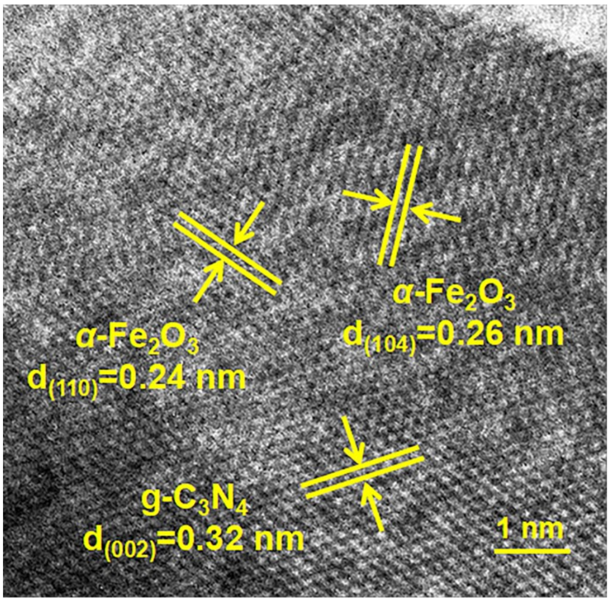

Figure S2. HRTEM image spectra of FOCN composite

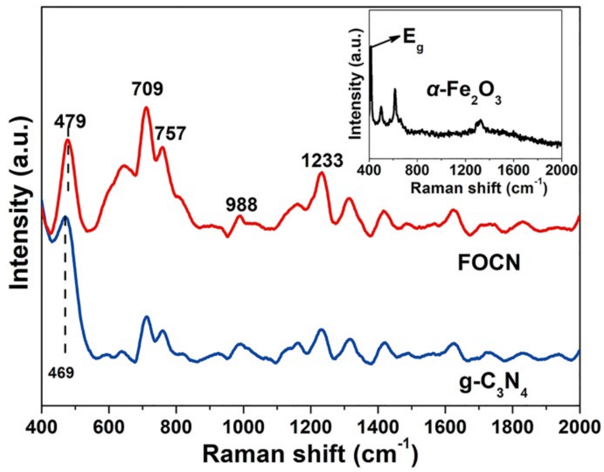

Figure S3. Raman spectra of pure g-C_3N_4, FOCN composites and α-Fe_2O_3.

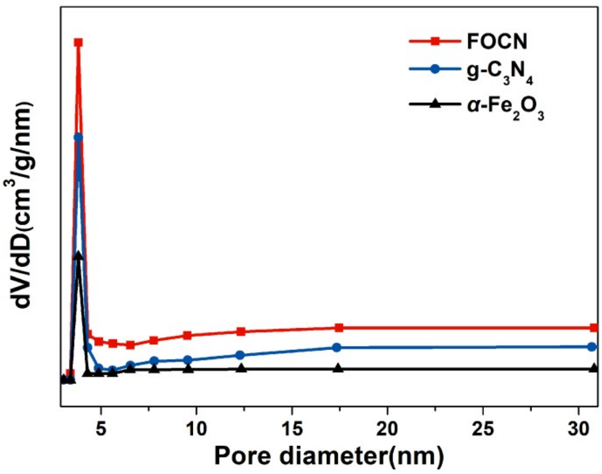

Figure S4. pore size distribution curves of g-C_3N_4, α-Fe_2O_3, and FOCN composite

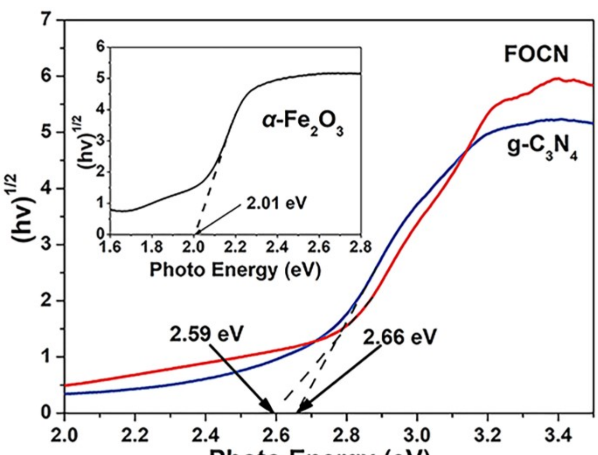

Figure S5. Estimated band gaps of pure g-C_3N_4, FOCN composite and α-Fe_2O_3.

E_{CB} of g-C_3N_4 and α-Fe_2O_3 could be calculated by the Mulliken electronegativity theory:

$$E_{CB}=X-E_C-0.5E_g \quad (1)$$

$$X=[X(A)^l X(B)^m X(C)^n]^{1/(l+m+n)} \quad (2)$$

$$E_{VB}=E_{CB}+E_g \quad (3)$$

Here, E_{CB} is the conduction band edge energy, X is the electronegativity of the semiconductor, Ec is the energy of free electrons with the hydrogen scale (4.50 eV), Eg is the band gap energy of the semiconductor[1]. So the values of E_{CB} and E_{VB} of α-Fe_2O_3 are determined to be 0.34 eV and 2.34 eV, respectively. The CB and VB edge potentials of g-C_3N_4 are at –1.14 eV and 1.52 eV, respectively[2]. The valence band (VB) and conduction band (CB) edge potentials of g-C_3N_4 and α-Fe_2O_3 were calculated according to Eqs. (1) ,(2) and (3).

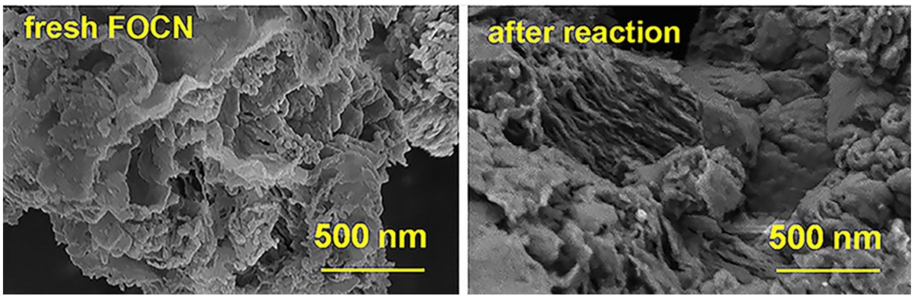

Figure S6. SEM image of FOCN composites before and after the photocatalytic reactions

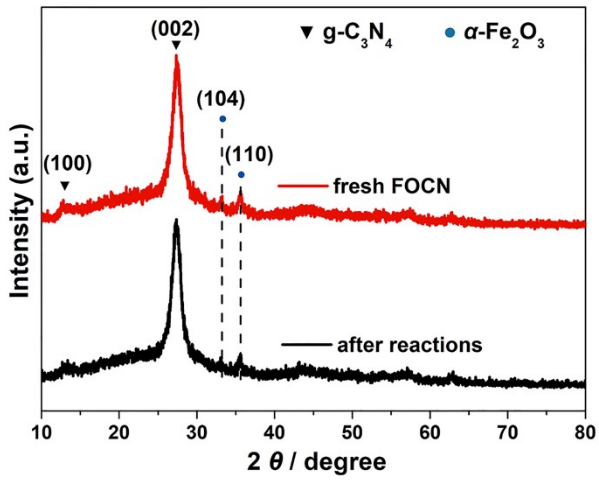

Figure S7. XRD patterns of FOCN composites before and after the photocatalytic reactions

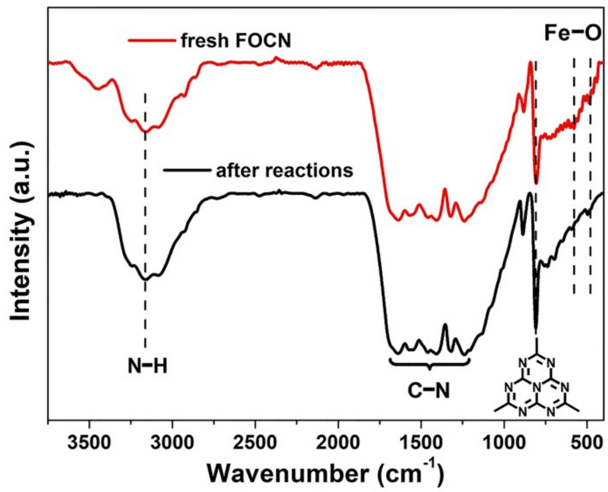

Figure S8. FT-IR spectra of FOCN composites before and after the photocatalytic reactions

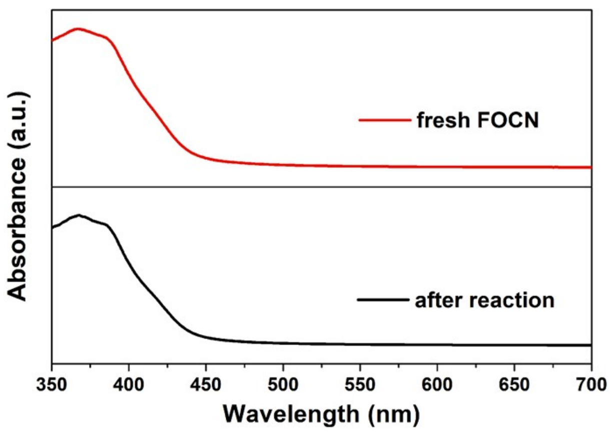

Figure S9 UV-vis spectra of FOCN composites before and after the photocatalytic reactions

Table S1. Summary of heterogeneous photocatalyzed Aza-Henry reaction.

Photocatalyst	Synthetic method	Light source	Solvent	Time	Yield	Ref.
CuO_2-MoS_2/graphene	precipitate method	24 W compact fluorescent bulb	nitromethane	8 h	79%	[1]
Cds	precipitate method	3 W LED	CH_3CN	24 h	97%	[2]
UiO-68Se	-	blue LED	CH_3NO_2	4 h	90%	[3]
TiO_2 or ZnO_2	-	11 W fluorescent bulb	EtOH	40 h	93%	[4]
In_2S_3/MoS_2	hydrothermal synthesis	20 W LED	nitromethane	24 h	74%	[5]
α-Fe_2O_3/g-C_3N_4	hydrothermal synthesis	50 W LED	nitromethane	24 h	62.7%	

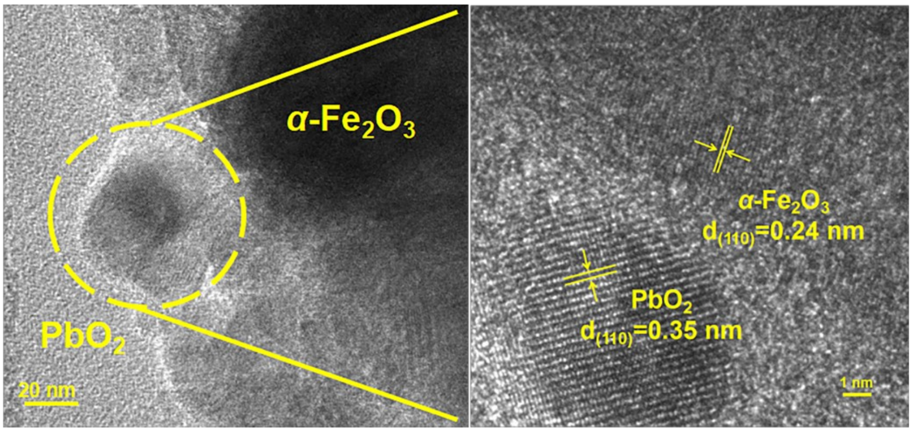

Figure S10 The TEM of photodeposition of composite materials

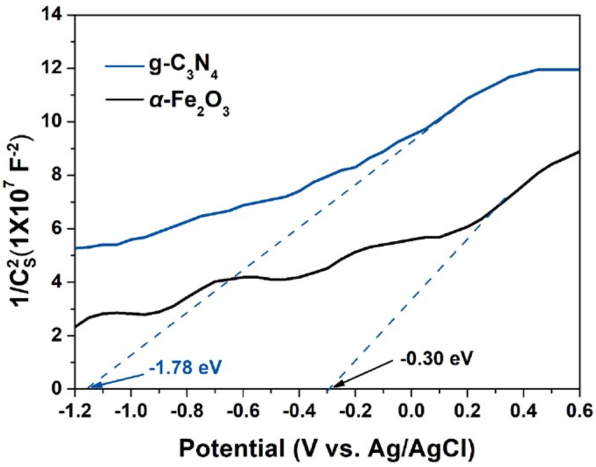

Figure S11 Mott-Schottky curves of g-C_3N_4 and α-Fe_2O_3

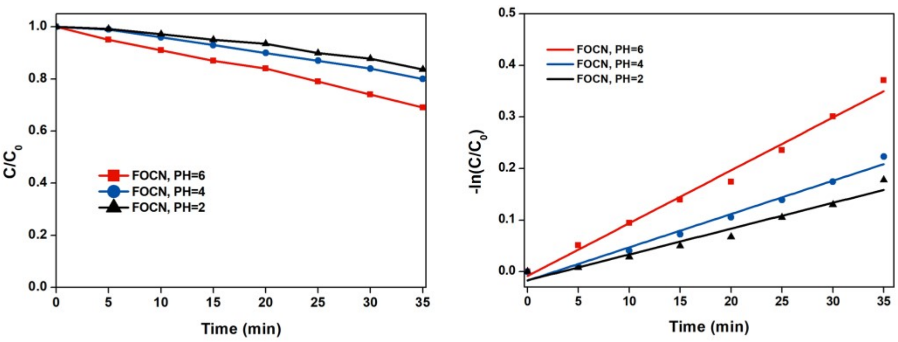

Figure S12 The activity of photocatalytic degradation of tetracycline with different pH

Process of photocatalytic degradation of tetracycline: 10 mg of FOCN was dispersed in 50 mL of tetracycline aqueous solution (50 ppm). After adsorption equilibrium, the mixture was stirred under the irradiation of a 300W Xe lamp for 35 min, and the concentration of tetracycline analyzed by UV–vis spectrophotometer.

The pH value of the system is around 6, due the intrinsic acidity of tetracycline aqueous solution. As shown in Figure S12, the photocatalytic degradation of tetracycline in FOCN system could be approximately fitted as a first order reaction. Note that, the decrease of pH value might decline the photocatalytic performance of FOCN.

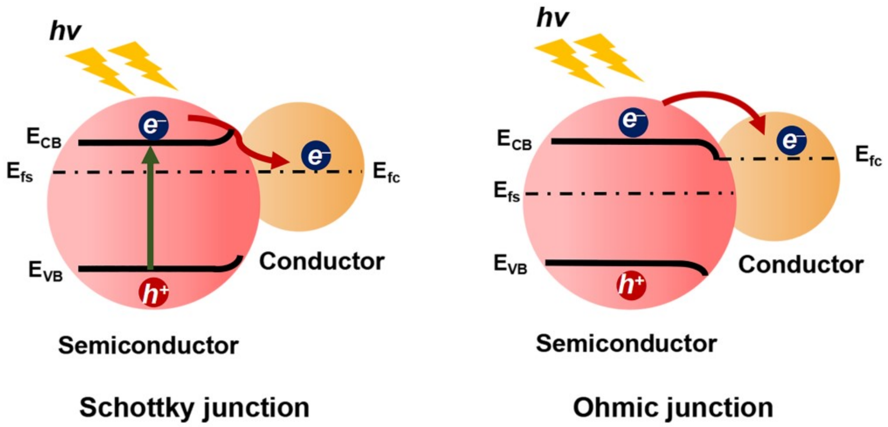

Figure S13 Design mechanism diagram from the band illustrating for the Schottky junction and the Ohmic contact of *n*-type semiconductor with the conductor.

When a semiconductor is combined with a conductor, them may form Schottky juntcion or Ohmic junction. Both Schottky junction and Ohmic junction accelerate spatial charge carrier separation and improve photocatalytic performance.

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