Supporting Information

Oxygen Self-doped g-C_3N_4 with Tunable Electronic Band Structure for Unprecedentedly Enhanced Photocatalytic Performance

Fangyan Wei,[a] Yang Liu,[a] Heng Zhao,[a] Xiaoning Ren,[a] Jing Liu,[a] Tawfique Hasan,[b] Lihua Chen,[a] Yu Li* [a] and Bao-Lian Su[a,c,d]

[a] *State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan University of Technology, 122 Luoshi Road, 430070, Wuhan, Hubei, China; Fax:+86 27 87879468; Tel: +86 27 87855322*

Email: yu.li@whut.edu.cn

[b] *Cambridge Graphene Centre, University of Cambridge, 9 JJ Thomson Avenue, Cambridge CB3 0FA, United Kingdom*

[c] *Laboratory of Inorganic Materials Chemistry, University of Namur, 61 rue de Bruxelles, B-5000 Namur, Belgium*

[d] *Clare Hall, University of Cambridge, Herschel Road, Cambridge CB3 9AL, United Kingdom*

Table S1. The molar mass of DCNA and CC.

samples	DCNA (mmol)	CC (mmol)	CC / DCNA
CNO-0.5	2.5	5	0.5
CNO-1	5	5	1
CNO-2	10	5	2
CNO-4	20	5	4

Table S2. XPS nitride spectra; peak area and N (SP^2)/N (SP^3) of N_1 peak.

samples	Relative peak area (%)				
	C-N=C	N-$(C)_3$	C-N-H	C=N	N (SP^2)/N (SP^3)
CN-Pure	70.0	16.4	10.7	2.9	4.26
CNO-1	59.4	31.7	8.9	0.0	1.87
CNO-2	52.9	32.2	14.9	0.0	1.64
CNO-4	59.0	30.6	10.4	0.0	1.93

Table S3. The atomic rate of C, N, Oand band gap for CN-Pure and CN-X samples.

samples	Atomic (%)					Band gap (eV)
	C	N	O	C/N	C : N : O	
CN-Pure	40.2	57.9	1.9	0.69	0.69:1:0.03	2.70
CNO-1	43.7	47.5	8.8	0.92	0.92:1:0.19	2.19
CNO-2	43.3	46.9	9.8	0.92	0.92:1:0.21	2.11
CNO-4	46.7	43.3	10.0	1.08	1.08:1:0.23	2.07

Table S4. XPS carbon spectra; peak area of C 1s peak.

Samples	Relative peak area(%)				
	C-C	C-O-C	N=C-N	C=N	C-O
CN-Pure	3.6	0.0	89.1	7.3	0.0
CNO-1	19.1	12.2	65.2	0.0	3.4
CNO-2	19.8	9.4	55.1	0.0	15.7
CNO-4	25.1	15.8	45.8	0.0	13.2

Table S5. XPS nitride spectra; peak area of N 1s peak.

sample	Relative peak area (%)			
	C-N=C	$N-(C)_3$	C-N-H	C=N
CN-Pure	70.0	16.4	10.7	2.9
CNO-1	59.4	31.7	8.9	0.0
CNO-2	52.9	32.2	14.9	0.0
CNO-4	59.0	30.6	10.4	0.0

Table S6. XPS oxygen spectra; peak area of O 1s peak

Sample	Relative peak area (%)			
	H_2O	O_2	C-O-C	N-C-O
CN-Pure	100.0			
CNO-1		2.2	21.4	76.4
CNO-2		3.2	13.0	83.8
CNO-4		5.3	20.5	74.2

Table S7. Pt loading on CN-pure and CNO-x (wt %)

Samples	CN-pure	CNO-0.5	CNO-1	CNO-2	CNO-4
Pt loading (wt %)	0.347	0.342	0.364	0.272	0.285

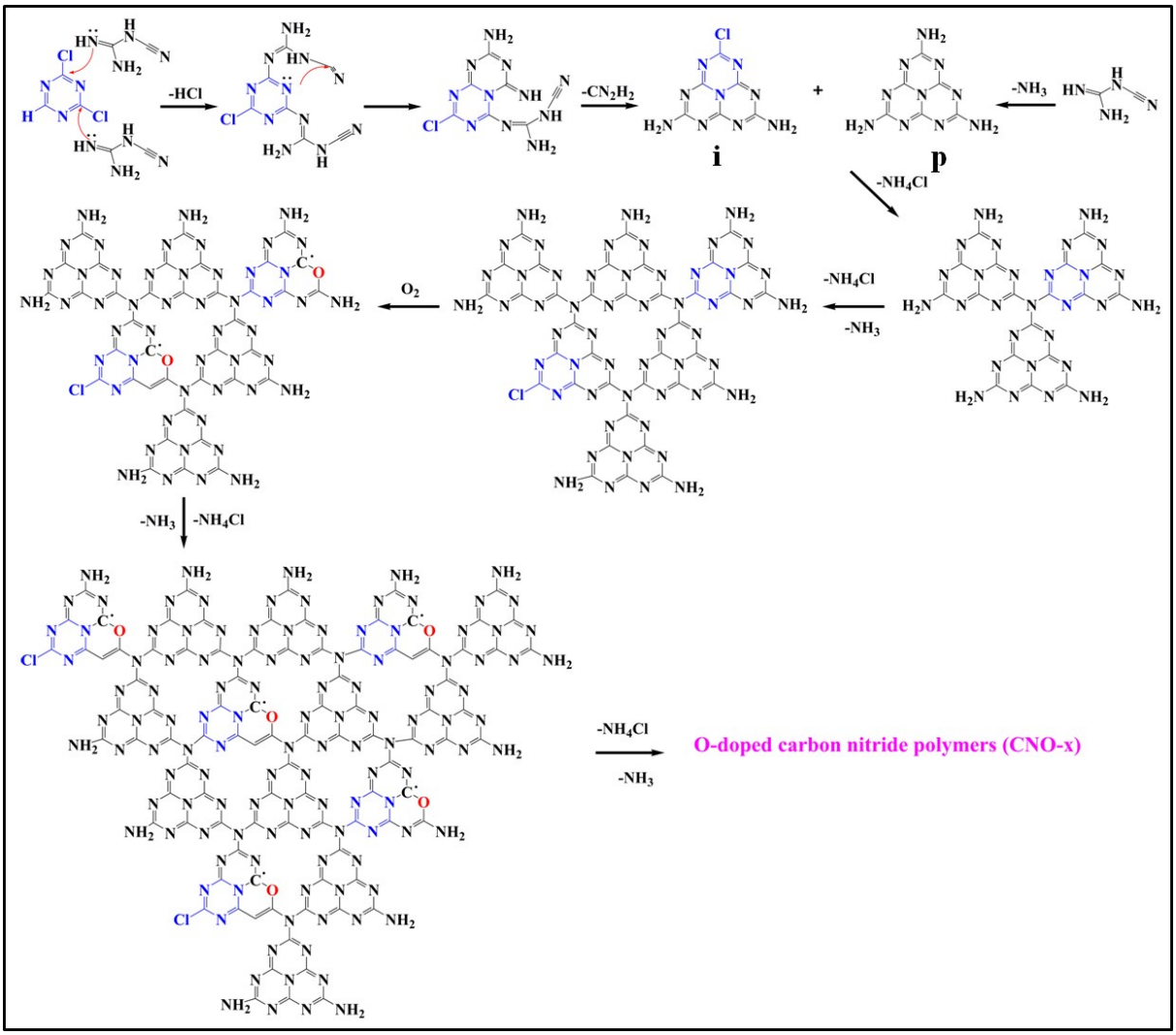

Figure S1. The copolymerization of dicyandiamide with 1,3,5-trichlorotriazine. The linkers can be integrated into the classic condensation process of oxygen self-doped g-C_3N_4 (CNO-x).

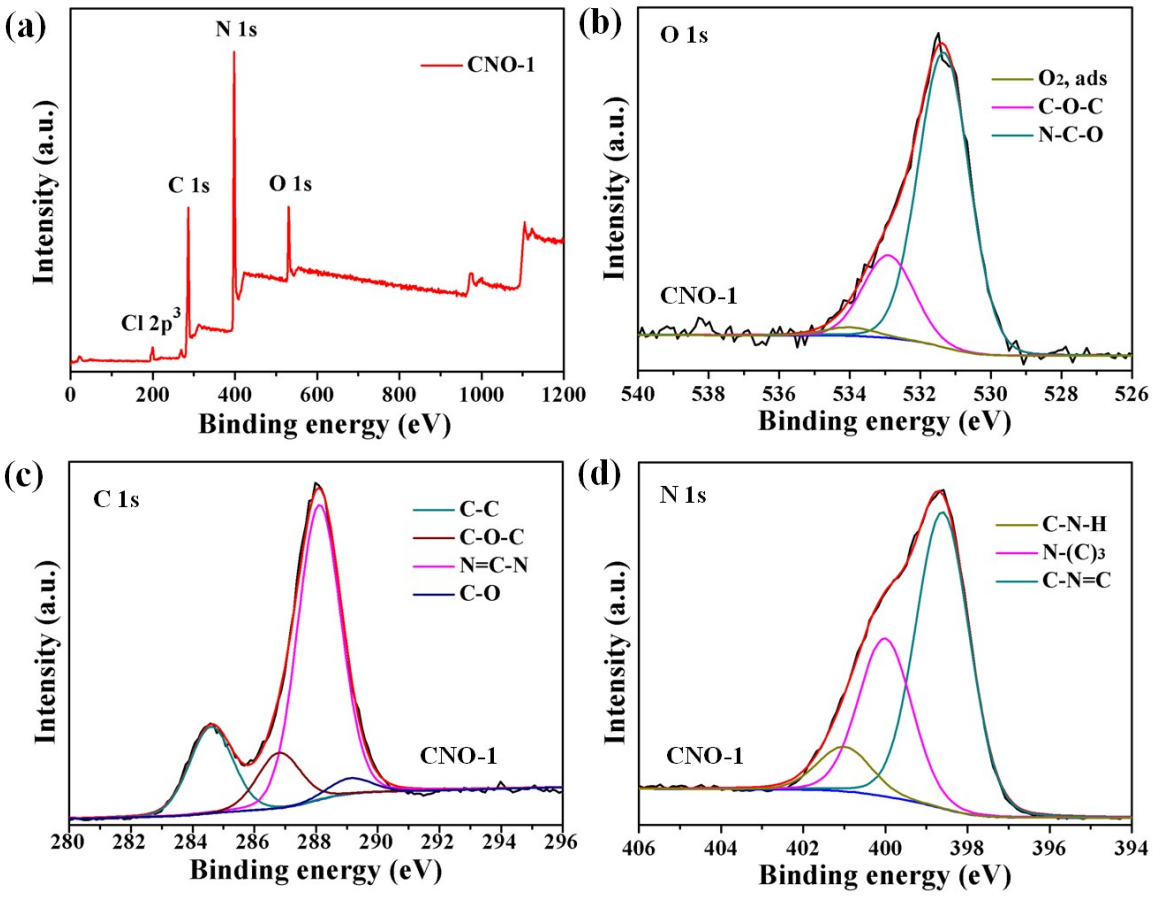

Figure S2. (a) XPS survey spectra and (b, c, d) High resolution O 1s, C 1s, N 1s XPS spectra of CNO-1.

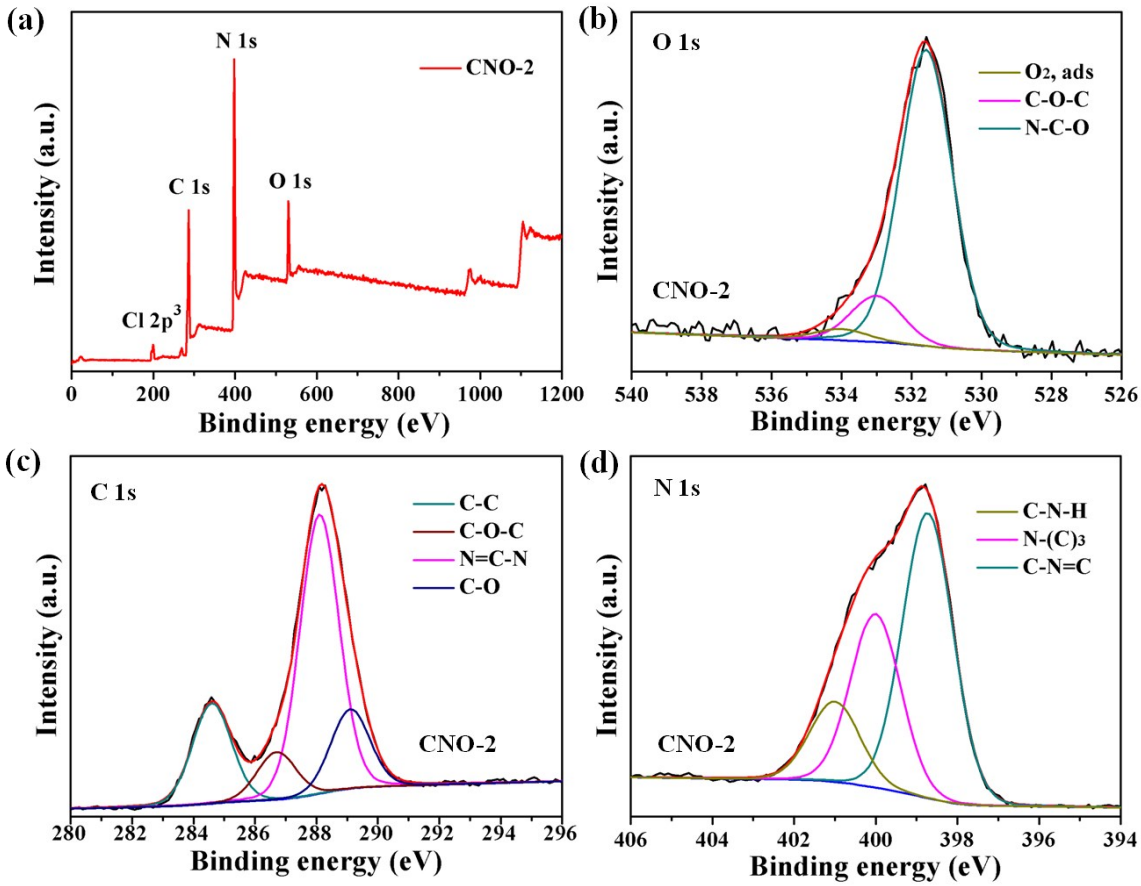

Figure S3. (a) XPS survey spectra and (b, c, d) High resolution O 1s, C 1s, N 1s XPS spectra of CNO-2.

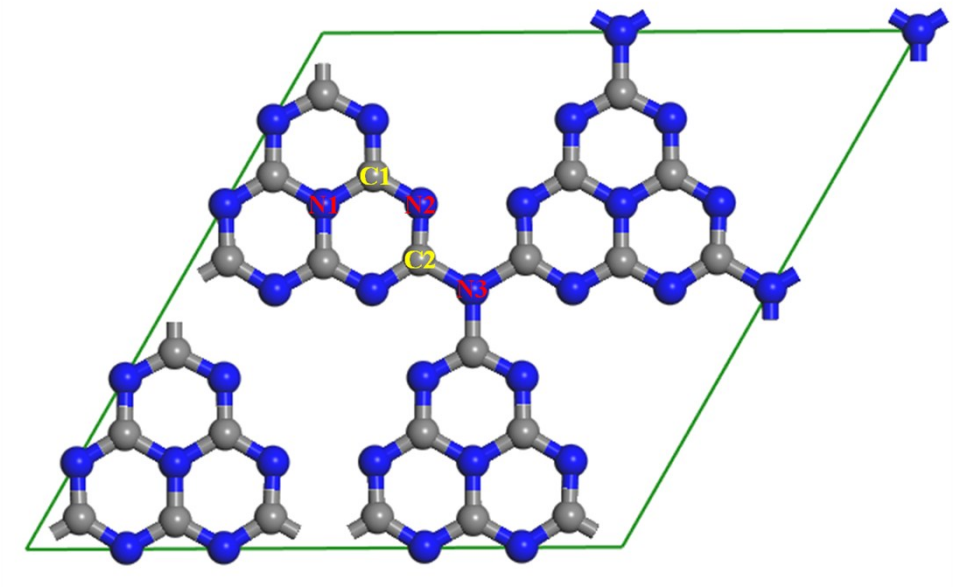

Figure S4. Structure of g-C_3N_4. The gray and blue spheres represent the carbon and nitrogen atoms, respectively, and different carbon and nitrogen atoms are labelled.

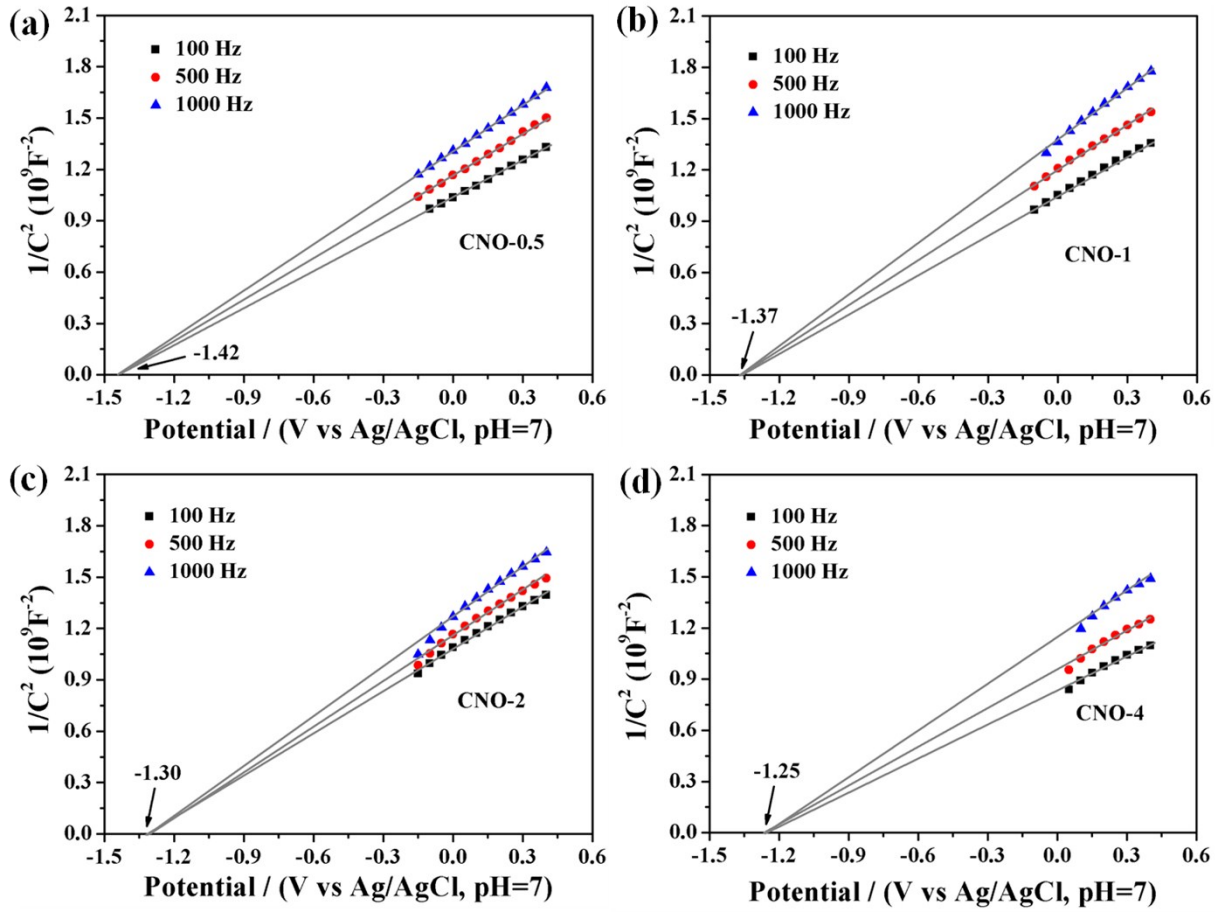

Figure S5. Mott–Schottky plots collected at various frequencies of (a) CNO-0.5, (b) CNO-1, (c) CNO-2 and (d) CNO-4.

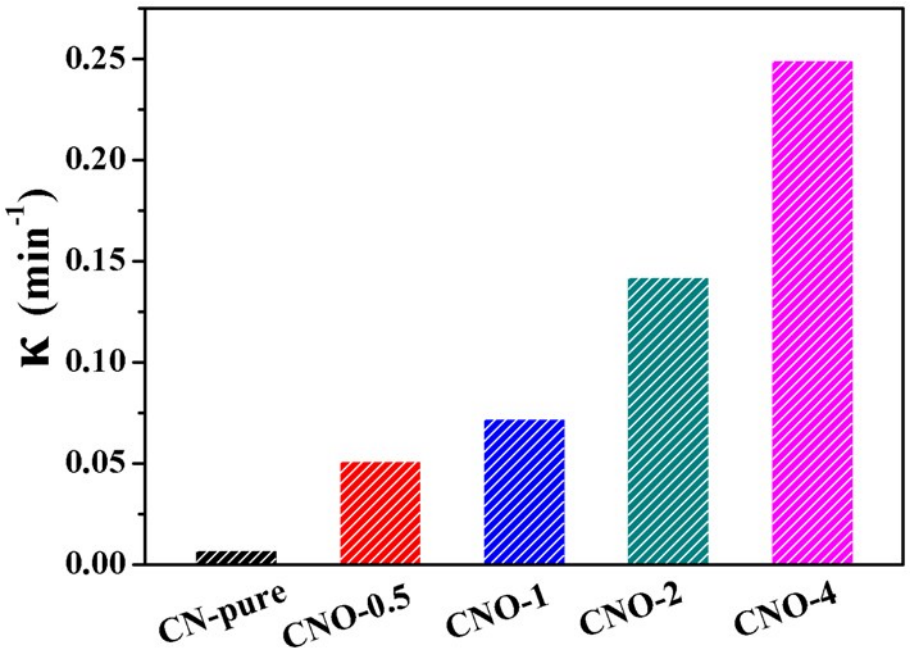

Figure S6. The rate constant of RhB degradation with different samples.