Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supplementary Information

One-step Construction of Y, C, and O Tridoped g-C_3N_4 as Bifunctional Photocatalyst for H_2 Evolution and Organic Pollutants Degradation under Visible Light Irradiation

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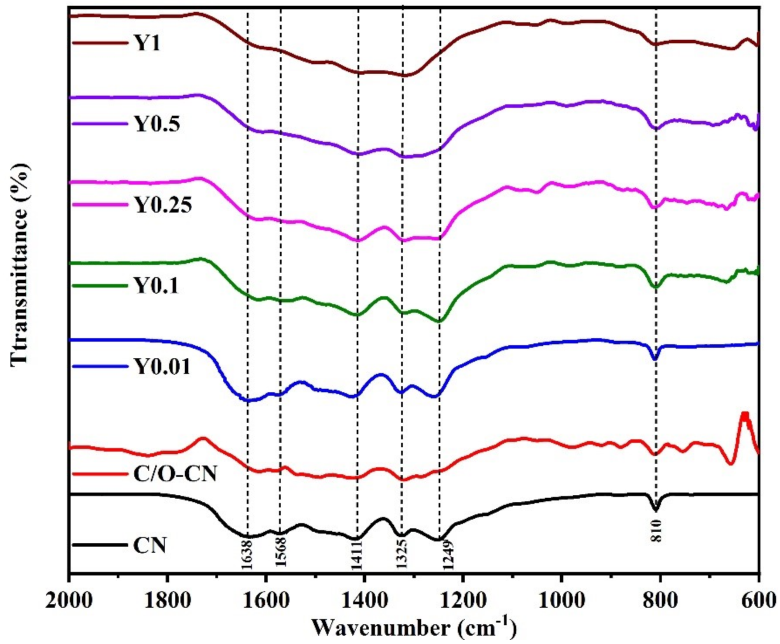

Fig. S1. FT-IR spectra in the range of 600 cm^{-1} to 2000 cm^{-1} of CN and doped CN samples.

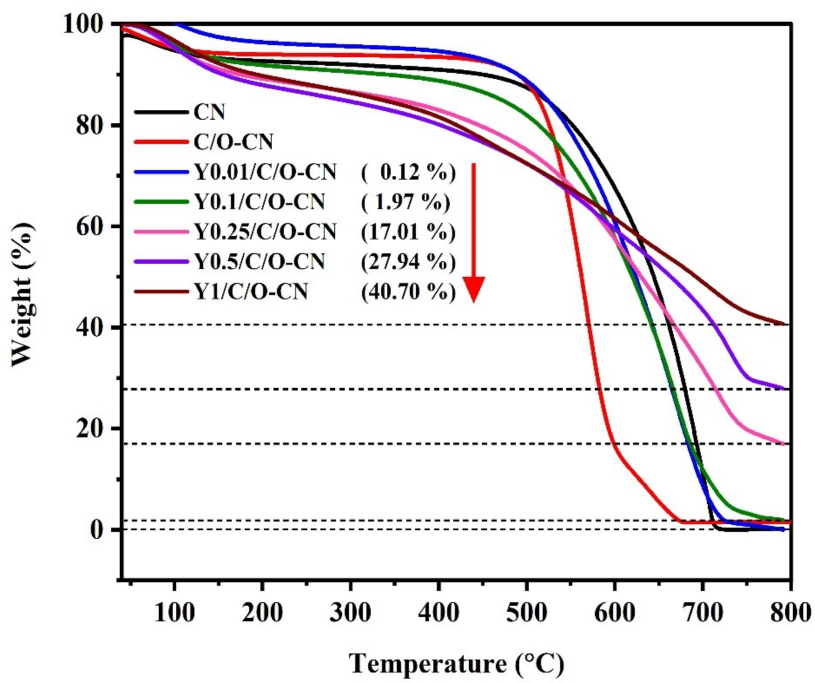

Fig. S2. TGA curves of bulk-CN, C/O-CN, and Yx/C/O tridoped CN samples.

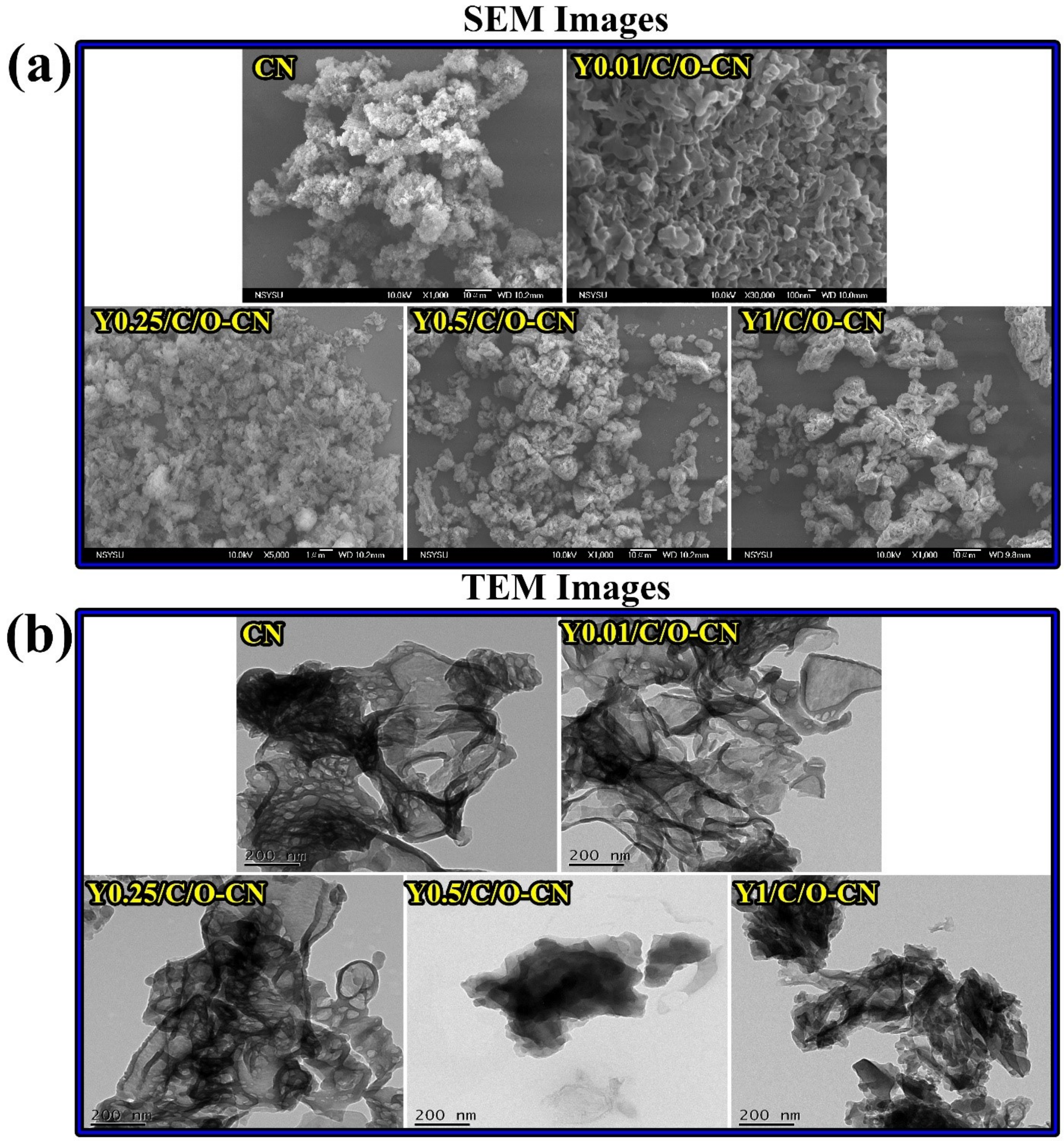

Fig. S3. (a) SEM images and (b) TEM images of bulk-CN and Yx/C/O tridoped CN samples.

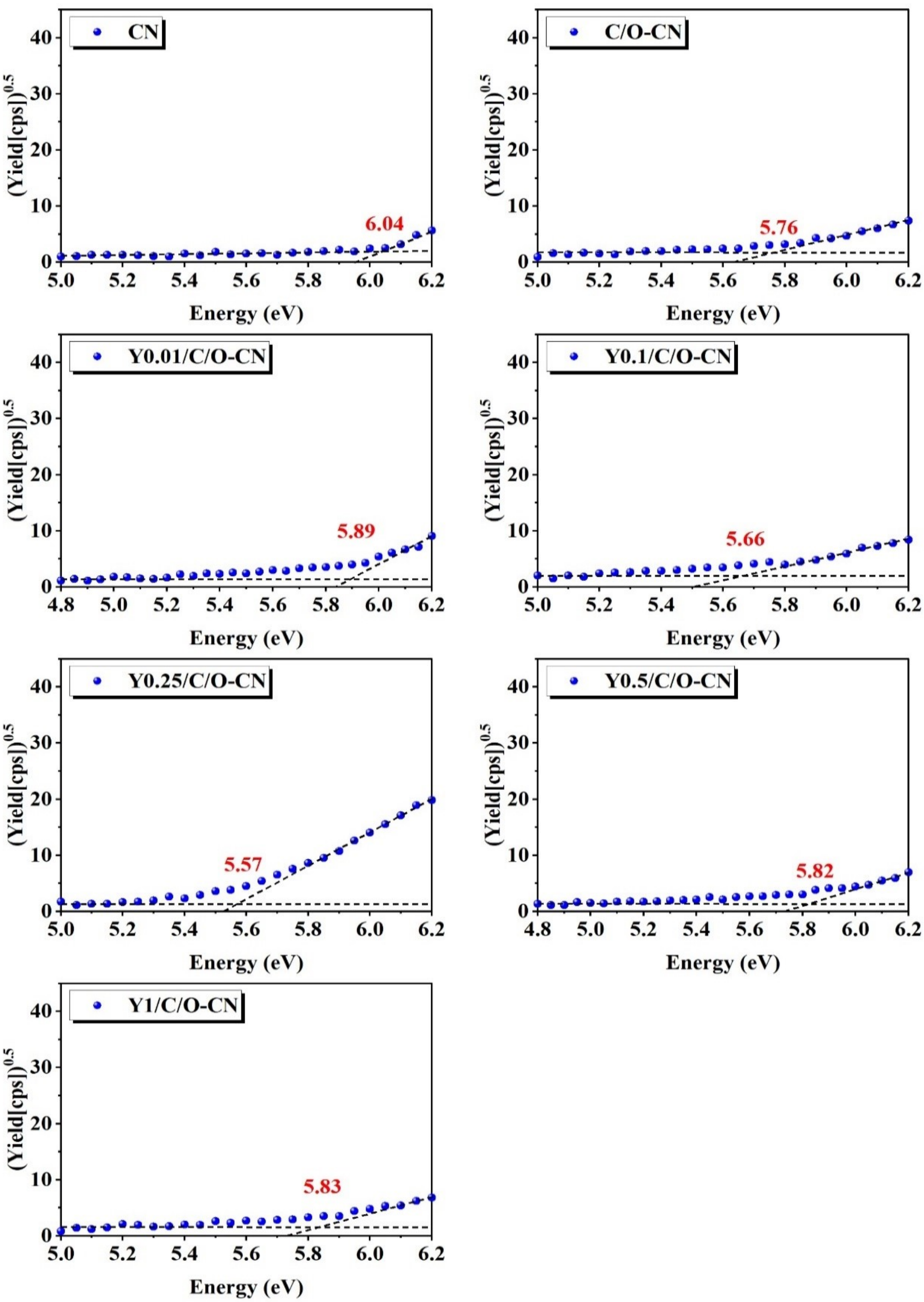

Fig. S4. Calculated valence band (VB) edges of CN and doped CN samples by photoelectron spectroscopy (model: AC-2).

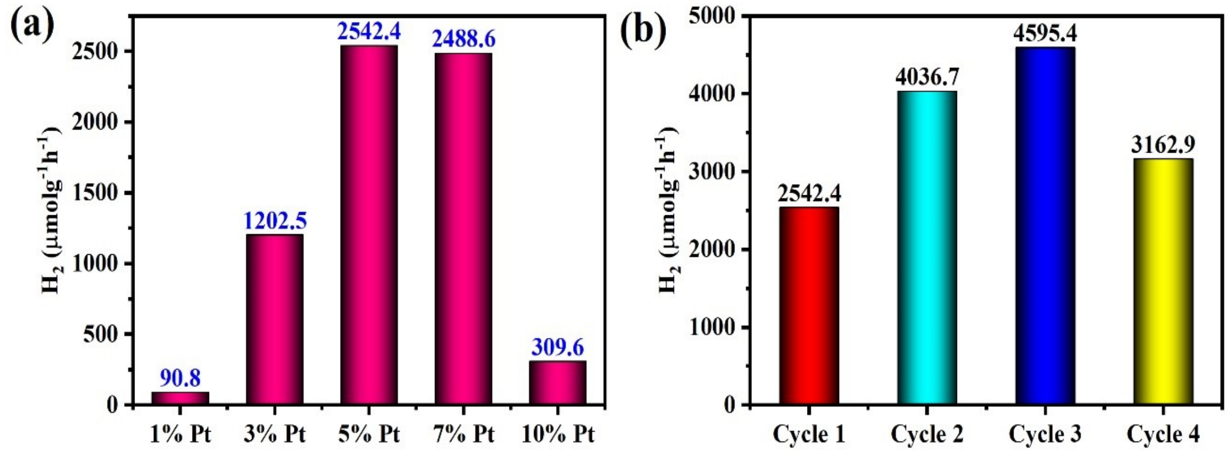

Fig. S5. (a) Effect of Pt co-catalyst concentration on photocatalytic H_2 evolution with Y0.1/C/O-CN and (b) stability test of Y0.1/C/O-CN for H_2 evolution.

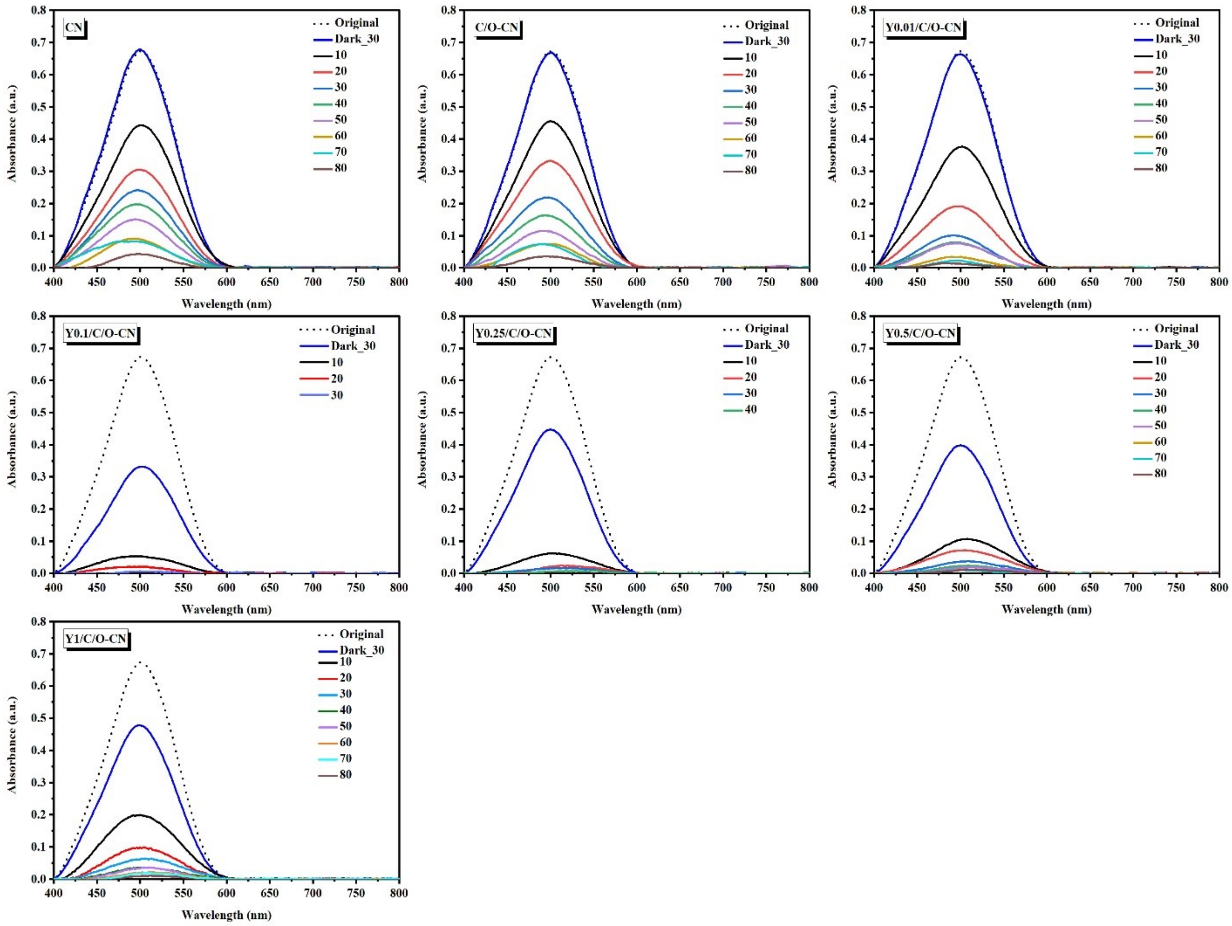

Fig. S6. The time-dependent absorption spectra of photocatalytic degradation of congo red (CR) dye under visible light irradiation with different photocatalysts.

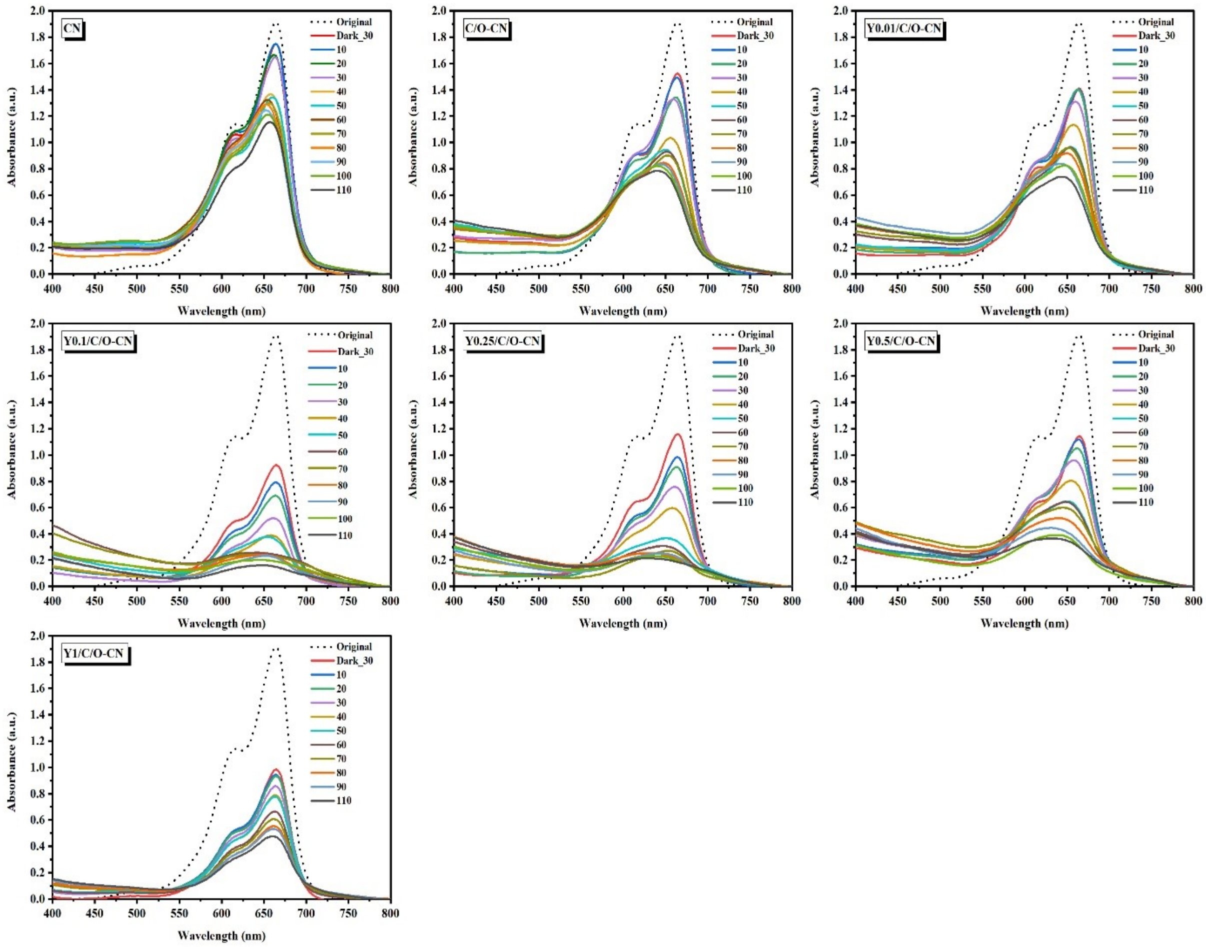

Fig. S7. The time-dependent absorption spectra of photocatalytic degradation of methylene blue (MB) dye under visible light irradiation with different photocatalysts.

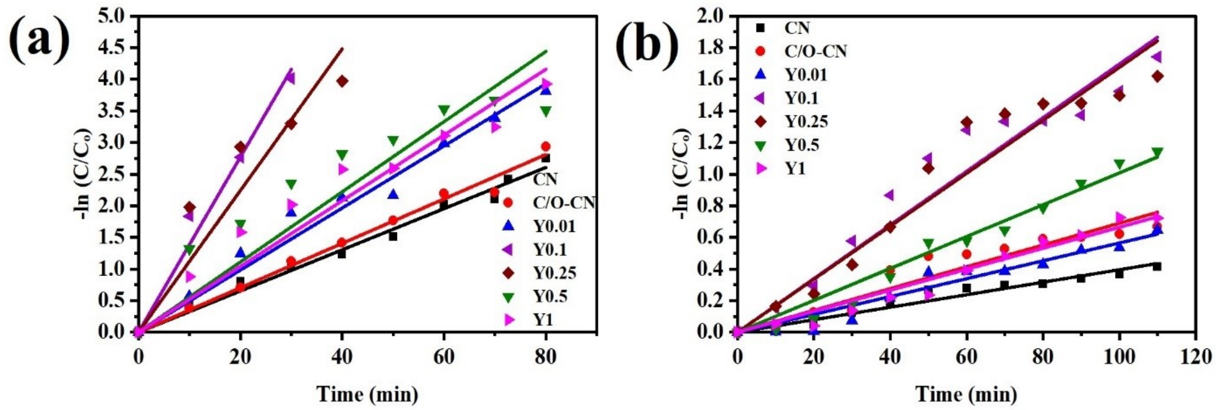

Fig. S8. -ln(C/C_o) versus reaction time plots for (a) CR and (b) MB degradation over bulk-CN, C/O-CN, and Yx/C/O tridoped CN, respectively.

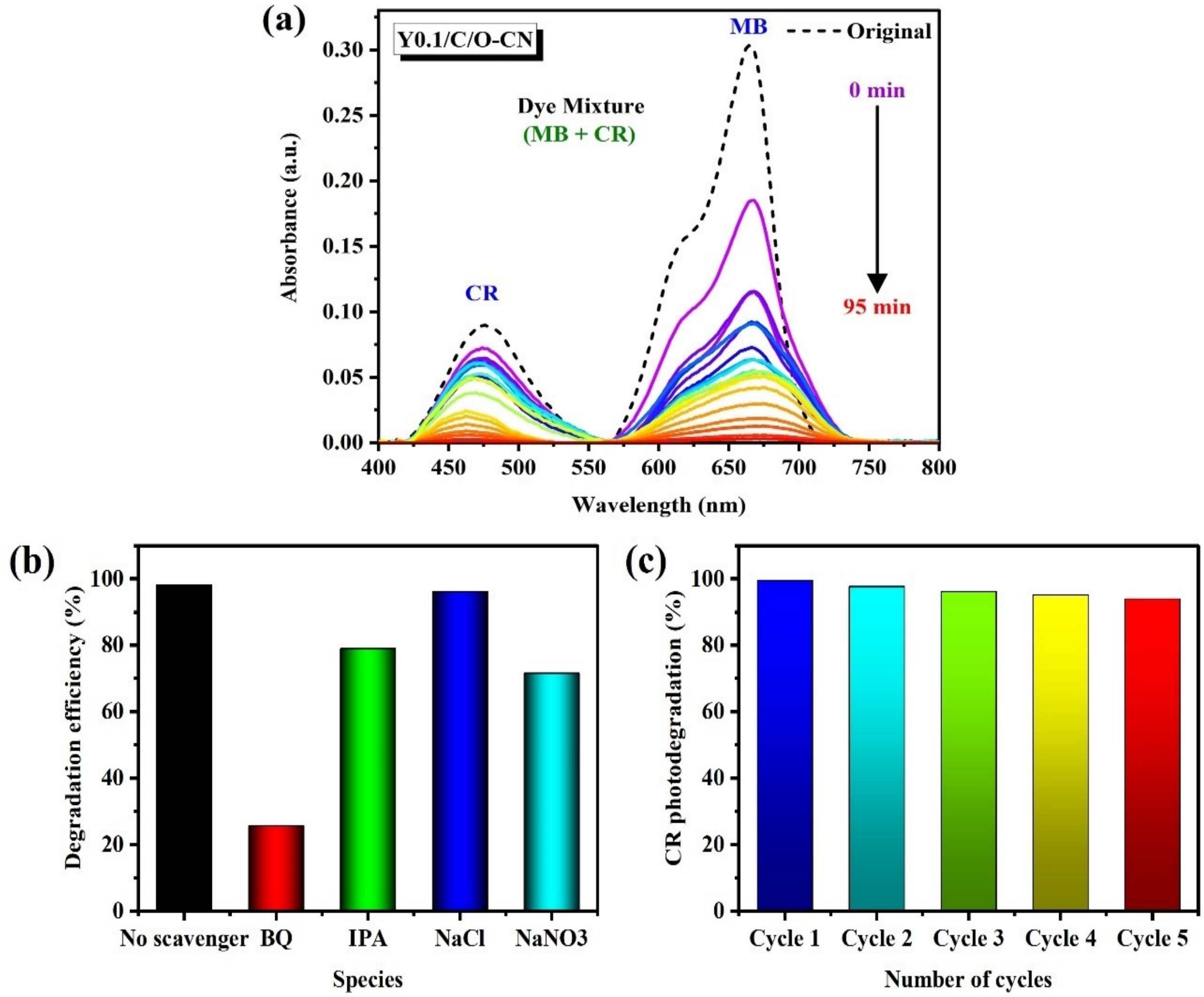

Fig. S9. (a) UV−visible absorbance of the model dye mixture (CR and MB) with the Y0.1/C/O-CN photocatalyst. (b) The effect of different scavengers on the CR photodegradation by Y0.1/C/O-CN, and (c) the reusability of Y0.1/C/O-CN photocatalyst for the degradation of CR.

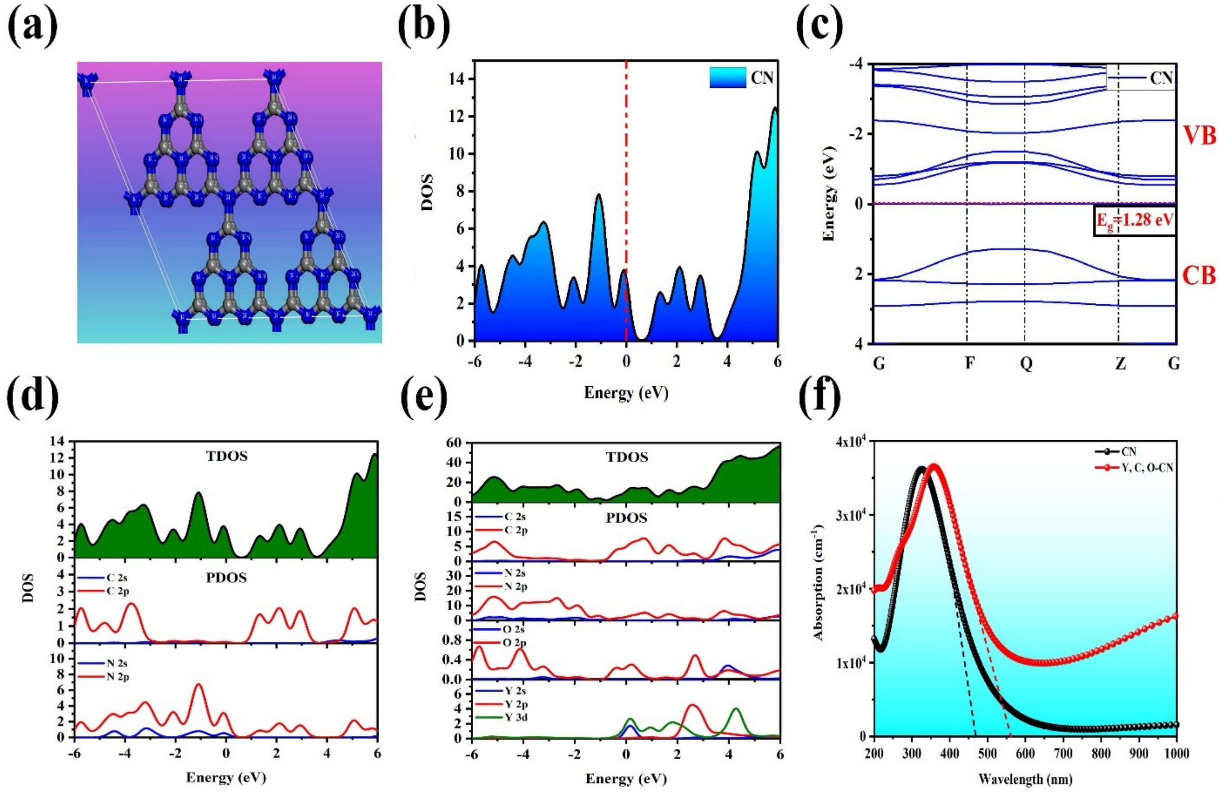

Fig. S10. (a) Optimized 2 × 2 × 1 supercell structure used in the DFT calculations, (b) calculated DOS diagram, and (c) corresponding band structure of pure CN, respectively. (d,e) TDOS and PDOS of pure CN and Y, C, O tridoped CN, respectively. (f) Optical absorption curve of pure CN and Y, C, O tridoped CN.

Table S1: XRD data information of CN and doped CN samples.

Samples	Average crystallite size (nm)	Dislocation density ($\times 10^{-19}$ m^{-2})	Lattice strain ($\times 10^{-2}$)
CN	2.569	1.529	1.353
C/O-CN	1.876	2.841	1.848
Y0.01/C/O-CN	2.053	2.372	1.688
Y0.1/C/O-CN	2.409	1.726	1.440
Y0.25/C/O-CN	2.059	2.402	1.694
Y0.5/C/O-CN	1.879	3.107	1.903
Y1/C/O-CN	1.557	4.375	2.271

Table S2: Surface elemental composition determined by XPS of pure-CN, C-O/CN, and Yx/C/O-CN samples.

Sample	**Atomic (%)**				**C/N ratio**
	C	**N**	**O**	**Y**	
g-C_3N_4 (CN)	44.13	53.91	1.970	-	0.819
C/O-CN	44.73	53.02	2.252	-	0.844
Y.01/C/O-CN	44.06	52.51	3.351	0.081	0.839
Y0.1/C/O-CN	43.10	51.23	5.030	0.640	0.841
Y0.25/C/O-CN	41.92	46.64	9.662	1.782	0.899
Y0.5/C/O-CN	41.48	42.83	12.66	3.020	0.968
Y1/C/O-CN	39.49	32.59	22.39	5.531	1.212

Table S3: XPS C 1s spectra results of CN, C/O-CN, and Y0.1/ C/O-CN.

Sample	**(N=C-$(N)_2$)**	**(C-C)**	**(C-O)**	**(N=C-$(N)_2$) / (C-C) ratio**
Pure-CN	88.4	10.2	1.4	8.65
C/O-CN	85.3	12.1	2.6	7.08
Y0.1/C/O-CN	85.4	12.7	1.9	6.71

Table S4: XPS N 1s spectra results of CN, C/O-CN, and Y0.1/ C/O-CN.

Sample	(C=N-C)	$(N\text{-}(C)_3)$	$(\text{-}NH_x)$
Pure-CN	59.6	29.2	11.2
C/O-CN	52.4	36.4	11.2
Y0.1/C/O-CN	48.9	39.4	11.7

Table S5: XPS O 1s spectra results of CN, C/O-CN, and Y0.1/ C/O-CN.

Sample	(H_2O)	(O_2)	(C-O)
Pure-CN	82.5	11.6	5.9
C/O-CN	58.4	25.1	16.5
Y0.1/C/O-CN	57.7	27.6	14.7

Table S6: BET surface area, pore size distribution, and bandgap energy (E_g) of pure-CN, C-O/CN, C/O-CN, and Yx/C/O-CN samples.

Sample	BET surface area (m^2/g)	Pore volume (cm^3/g)	Bandgap (eV)
g-C_3N_4 (CN)	62.07	0.054	2.75
C/O-CN	36.91	0.034	1.86
Y.01/C/O-CN	43.47	0.051	1.88
Y0.1/C/O-CN	80.39	0.112	1.90
Y0.25/C/O-CN	73.90	0.125	2.11
Y0.5/C/O-CN	46.35	0.123	2.15
Y1/C/O-CN	28.76	0.119	2.27

Table S7: Comparison of photocatalytic activity of Yx/C/O tridoped g-C_3N_4 (x= 0.01, 0.1, 0.25, 0.5, and 1 g) for H_2 evolution and the corresponding AQY with other g-C_3N_4 based photocatalysts.

Photocatalyst	Experimental details	Light source	HER (μmol h^{-1} g^{-1})	AQY (%) (420nm)	Ref.
g-C_3N_4-Based Heterojunction Photocatalysts					
N-doped MoS_2/ S-doped g-C_3N_4	Water/ TEOA/ Pt	300 W Xe lamp (>420 nm)	659	-	1
CdS QDs/ P-doped g-C_3N_4	Water/ Na_2S/ Na_2SO_3	300 W Xe lamp (>420 nm)	1579	-	2
B-doped g-C_3N_4/ ZnO	Water/ TEOA/ Pt	300 W Xe lamp (>420 nm)	357	3.29 (240 nm)	3
Monodoped g-C_3N_4 Photocatalysts					
S-doped g-C_3N_4 nanosheets	Water/ TEOA/ Pt	300 W Xe lamp (>420 nm)	982	-	4
Br-doped g-C_3N_4	Water/ TEOA/ Pt	300 W Xe lamp (>420 nm)	960	-	5
Cl-doped g-C_3N_4	Water/ lactic acid/ Pt	300 W Xe lamp (>420 nm)	537	13.7	6
P-doped g-C_3N_4	Water/ TEOA/ Pt	300 W Xe lamp (>420 nm)	1596	3.6	7
C-doped g-C_3N_4	Water/ TEOA/ Pt	300 W Xe lamp (>400 nm)	178	-	8
F-doped g-C_3N_4	Water/ TEOA/ Pt	300 W Xe lamp (>420 nm)	745	-	9
O-doped porous network g-C_3N_4	Water/ TEOA/ Pt	300 W Xe lamp (>420 nm)	1204	7.8	10
O-doped porous g-C_3N_4	Water/ TEOA/ Pt	300 W Xe lamp (>420 nm)	1430	-	11
O-doped g-C_3N_4	Water/ TEOA/ Pt	300 W Xe lamp (>420 nm)	772	8.6	12

K-doped g-C_3N_4	Water/ TEOA/ Pt	300 W Xe lamp (>420 nm)	1028	-	13
		Codoped g-C_3N_4 Photocatalysts			
Mo-S codoped porous g-C_3N_4 nanosheets	Water/ TEOA/ Pt	300 W Xe lamp (>420 nm)	294	0.24	14
P-Na codoped g-C_3N_4	Water/ TEOA/ Pt	300 W Xe lamp (>400 nm)	2032	6.8	15
Fe-P codoped g-C_3N_4	Water/ methanol / Pt	250 W Na lamp (>400 nm)	122	6.9	16
C-O codoped g-C_3N_4	Water/ TEOA/ Pt	300 W Xe lamp (>420 nm)	1101	-	This work
		Tridoped g-C_3N_4 Photocatalysts			
S-P-O tridoped g-C_3N_4 nanosheet	Water/ TEOA/ Pt	300 W Xe lamp (>420 nm)	2480	-	17
Y0.01-C-O tridoped g-C_3N_4	Water/ TEOA/ Pt	300 W Xe lamp (>420 nm)	2212	-	This work
Y0.1-C-O tridoped g-C_3N_4	**Water/ TEOA/ Pt**	**300 W Xe lamp (>420 nm)**	**2543**	**6**	**This work**
Y0.25-C-O tridoped g-C_3N_4	Water/ TEOA/ Pt	300 W Xe lamp (>420 nm)	958	-	This work
Y0.5-C-O tridoped g-C_3N_4	Water/ TEOA/ Pt	300 W Xe lamp (>420 nm)	335	-	This work
Y1-C-O tridoped g-C_3N_4	Water/ TEOA/ Pt	300 W Xe lamp (>420 nm)	59	-	This work

Table S8: Comparison of photocatalytic activity of Yx/C/O tridoped g-C_3N_4 (x= 0.01, 0.1, 0.25, 0.5, and 1 g) for pollutant degradation with other g-C_3N_4 based photocatalyst.

Photocatalyst	Catalyst dose (g/L)	Dye Used	Dye Conc. (ppm)	Light source	Degradation (%)	Time (min)	Ref.
			CR Photodegradation				
S-doped g-C_3N_4/TiO_2	0.2	CR	50	300 W Xe lamp	95	60	18
g-C_3N_4/RGO/$Bi_2Fe_4O_9$	0.5	CR	10	30 W LED lamp (>420 nm)	87.7	60	19
$CoFe_2O_4$/g-C_3N_4 *(In the presence of 30%H_2O_2)*	0.5	CR	25	150 W Xe lamp simulated solar light	~100%	90	20
Exfoliated g-C_3N_4	1	CR	100	Solar irradiation	95.1	60	21
g-C_3N_4/precipitated silica	2	CR	60	300 W Xe lamp (>400 nm)	88	360	22
Acid-etched template free g-C_3N_4	0.05	CR	10	Visible light	90.08	150	23
C-O codoped g-C_3N_4	0.2	CR	50	18 W LED lamp (>420 nm)	94.7	80	This work
Y0.01-C-O tridoped g-C_3N_4	0.2	CR	50	18 W LED lamp (>420 nm)	97.8	80	This work
Y0.1-C-O tridoped g-C_3N_4	**0.2**	**CR**	**50**	**18 W LED lamp (>420 nm)**	**98.5**	**30**	**This work**
Y0.25-C-O tridoped g-C_3N_4	0.2	CR	50	18 W LED lamp (>420 nm)	98.1	40	This work
Y0.5-C-O tridoped g-C_3N_4	0.2	CR	50	18 W LED lamp (>420 nm)	97.0	80	This work
Y1-C-O tridoped g-C_3N_4	0.2	CR	50	18 W LED lamp (>420 nm)	98.0	80	This work
			MB Photodegradation				
Li-doped g-C_3N_4	0.2	MB	30	300 W Xe lamp (>470 nm)	90	180	24
Ca-doped $NaNbO_3$/g-C_3N_4	0.4	MB	1	85 W CFL lamp	100	240	25
ZnO/Au/g-C_3N_4	0.5	MB	10	300 W Xe lamp	99	120	26
g-C_3N_4/H-ZSM-5	0.1	MB	5	None	92	120	27

$g-C_3N_4/RGO/Bi_2Fe_4O_9$	0.5	MB	10	30 W LED (>420 nm)	87.7	60	19
UiO-66/$g-C_3N_4$	0.25	MB	10	350 W Xe lamp (>420 nm)	~100	240	28
Sm_2O_3/S-doped $g-C_3N_4$	0.7	MB	8	300 W Halogen lamp (>400 nm)	93	150	29
Porous CeO_2/S-doped $g-C_3N_4$	-	MB	7	300 W Halogen lamp (>400 nm)	91	150	30
ZnS/$g-C_3N_4$	0.15	MB	6	100 W Halogen lamp	90	100	31
$g-C_3N_4/Cu_2O$	0.5	MB	3.1	400 W Na lamp	81	120	32
C-O codoped $g-C_3N_4$	0.2	MB	10	18 W LED lamp (>420 nm)	48.6	110	This work
Y0.01-C-O tridoped $g-C_3N_4$	0.2	MB	10	18 W LED lamp (>420 nm)	47.6	110	This work
Y0.1-C-O tridoped $g-C_3N_4$	**0.2**	**MB**	**10**	**18 W LED lamp (>420 nm)**	**82.4**	**110**	**This work**
Y0.25-C-O tridoped $g-C_3N_4$	0.2	MB	10	18 W LED lamp (>420 nm)	80.2	110	This work
Y0.5-C-O tridoped $g-C_3N_4$	0.2	MB	10	18 W LED lamp (>420 nm)	68.1	110	This work
Y1-C-O tridoped $g-C_3N_4$	0.2	MB	10	18 W LED lamp (>420 nm)	51.5	110	This work
				Mixed Dyes Photodegradation			
Y0.1-C-O tridoped $g-C_3N_4$	**0.2**	**MB, CR**	**10, 25**	**18 W LED lamp (>420 nm)**	**~100**	**95**	**This work**
$CoFe_2O_4/g-C_3N_4$ *(In the presence of 30%H_2O_2)*	0.5	MB, CR, MO	25, 25, 10	150 W Xe lamp simulated solar light	~100	180	20

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