

Electronic supplementary information

Molecular p-n heterojunction-enhanced visible-light hydrogen evolution over N-doped TiO₂ photocatalyst

Liming Chen,^{a,b} Quan Gu,^c Linxi Hou,^{b*} Chaoqiang Zhang,^a Yinbing Lu,^a Xuxu Wang^a and Jinlin Long^{a*}

^a Research Institute of Photocatalysis, State Key Laboratory of Photocatalysis on Energy and Environment, College of Chemistry, Fuzhou University, Fuzhou, 350002, People's Republic of China

^b Department of Materials-Oriented Chemical Engineering, College of Chemical Engineering, Fuzhou University, Fuzhou, 350108, People's Republic of China

^c Key Laboratory of Applied Surface and Colloid Chemistry, Ministry of Education, School of Chemistry and Chemical Engineering, Shaanxi Normal University, Xi'an, 710062, People's Republic of China

Table of Contents

1	Figure S1.	Page S2
2	Figure S2.	Page S2
3	Figure S3.	Page S2
4	Figure S4.	Page S3
5	Figure S5.	Page S3
6	Figure S6.	Page S4
7	Table S1.	Page S5
8	Table S2.	Page S6

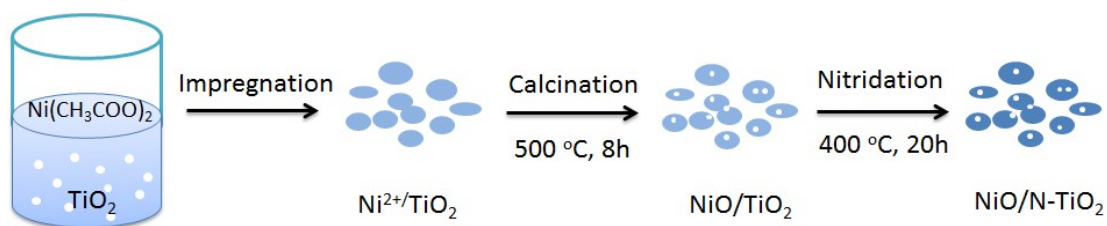


Figure S1. The preparation process of the NiO coupled N doped TiO_2 samples

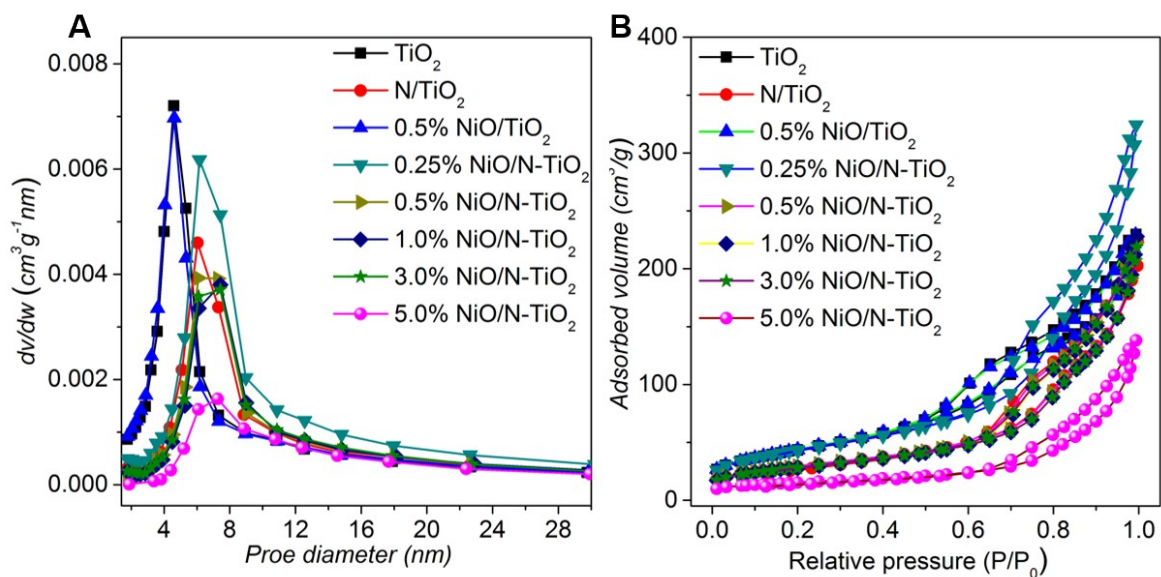


Figure S2. (A) The nitrogen adsorption-desorption isotherms and (B) the corresponding pore-size distribution curves of samples.

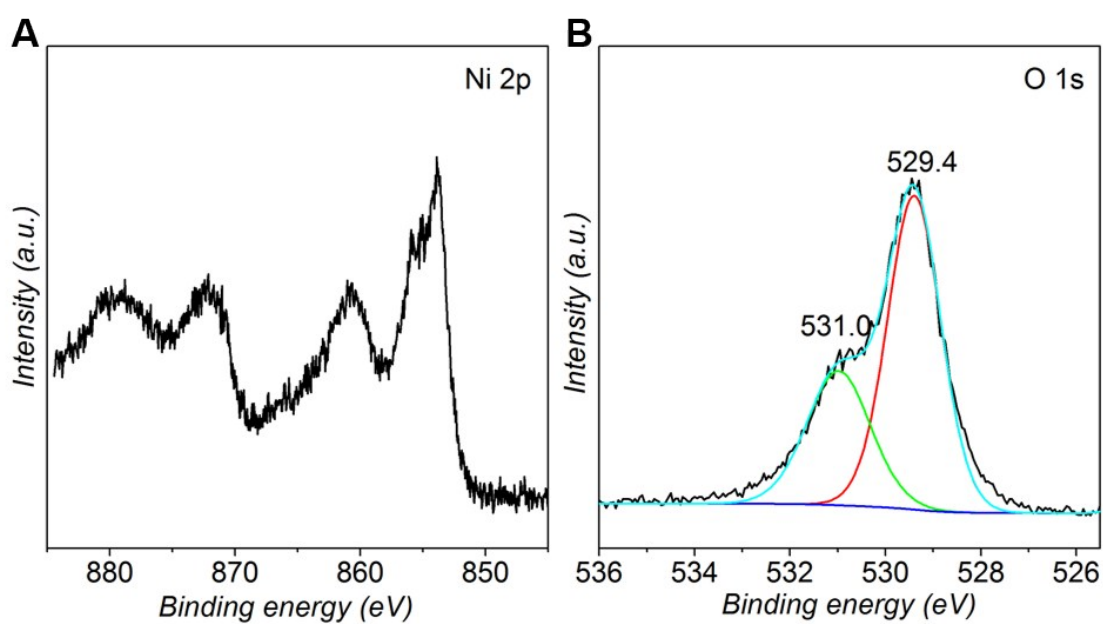


Figure S3. The high resolution core XPS spectra of Ni 2p and O 1s of bare NiO nanoparticles.

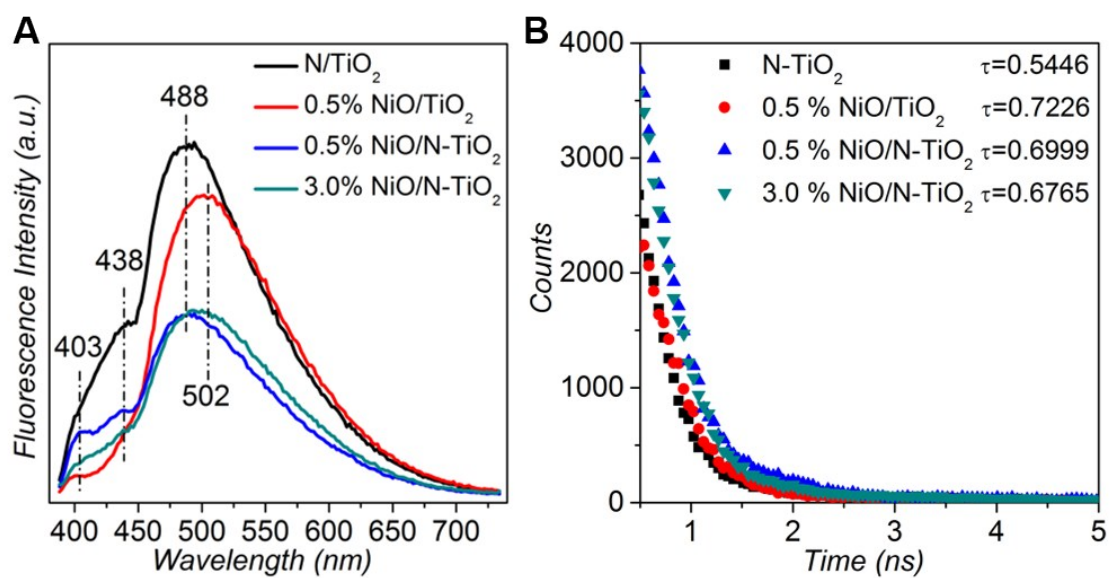


Figure S4. (A) PL emission spectra of N-TiO₂, 0.5 wt% NiO/TiO₂, 0.5 wt% NiO/N-TiO₂ and 3.0 wt% NiO/N-TiO₂ samples with excitation wavelength of 380 nm. (B) Time-resolved PL decays of samples.

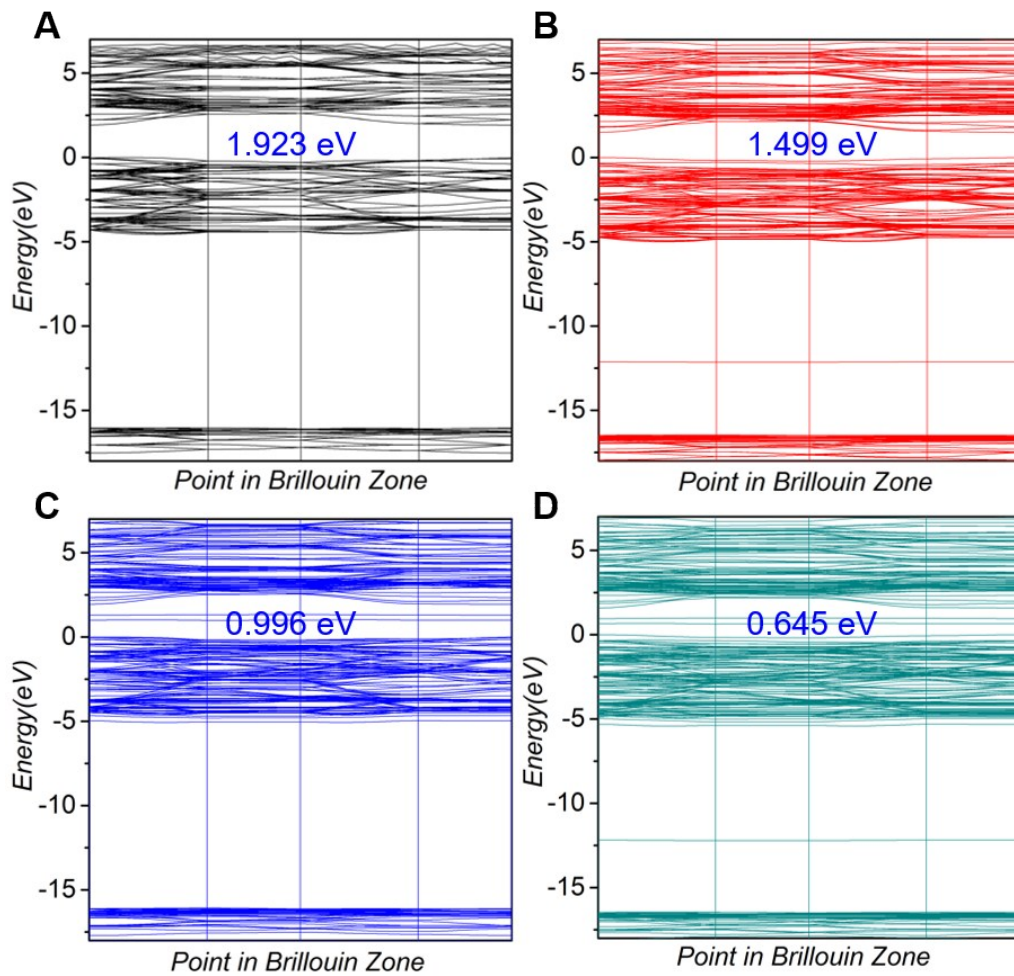


Figure S5. The band structure of (A) TiO_2 , (B) N- TiO_2 , (C) N- TiO_2 and (D) NiO/N- TiO_2 photocatalysts.

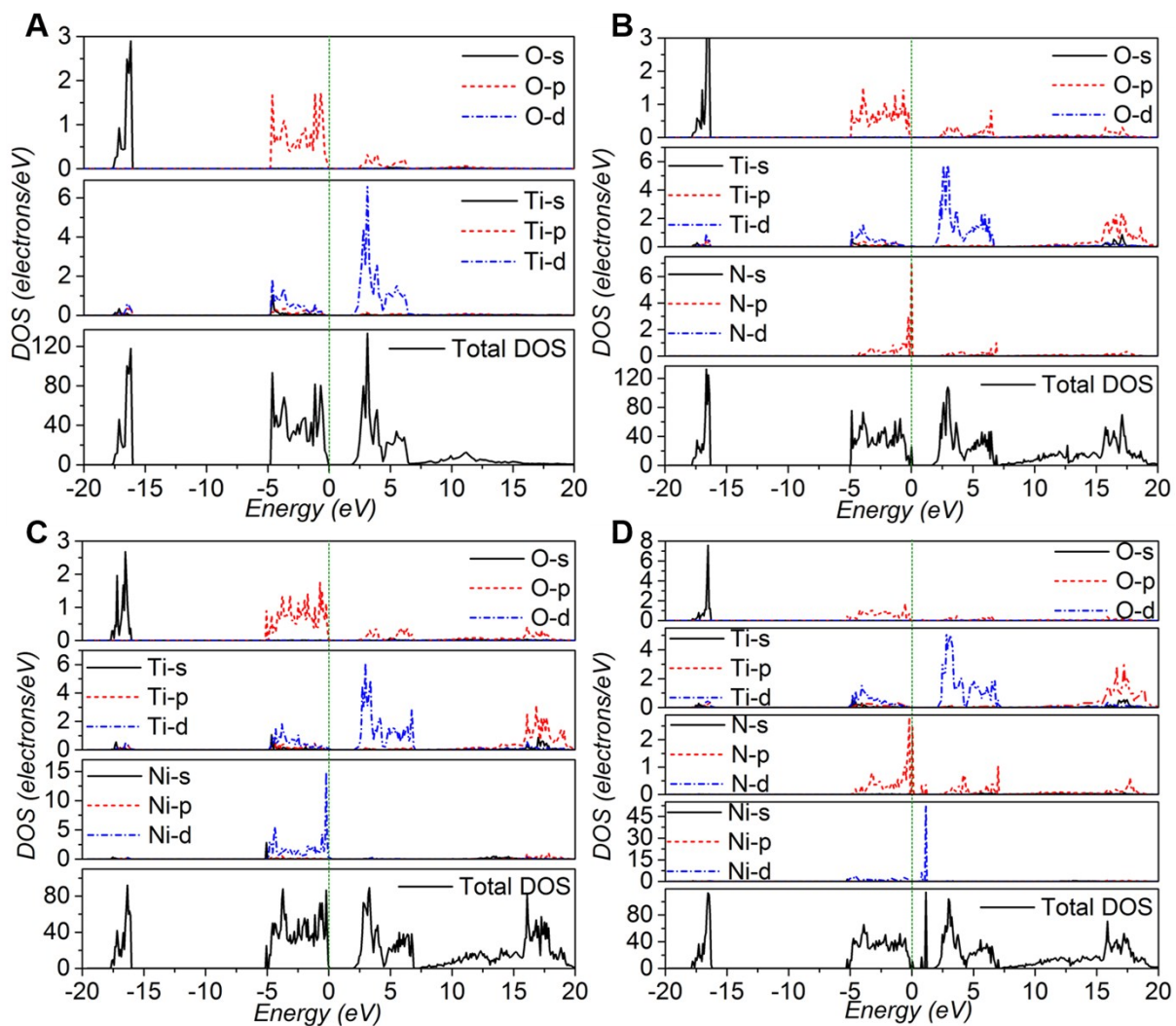


Figure S6. The density of states (DOS) of (A) TiO_2 , (B) N-TiO_2 , (C) N-TiO_2 and (D) NiO/N-TiO_2 photocatalysts.

Table S1. Physicochemical Characteristics of TiO₂, N-TiO₂, 0.5 wt% NiO/TiO₂ and x wt% NiO/N-TiO₂ samples.

Sample	N wt%	Ni wt%	Ni/N	Pore Volume (mL/g)	Pore Size (nm)	S _{BET} (m ² /g)
TiO ₂	-	-	-	0.3606	6.90	159.0
N/TiO ₂	0.77	-	-	0.3352	9.60	111.4
0.5%NiO/TiO ₂	0	0.53	-	0.3604	6.97	160.4
0.25%NiO/N-TiO ₂	0.77	0.27	0.084	0.5049	10.29	107.8
0.35%NiO/N-TiO ₂	0.77	0.39	0.124	0.3525	10.62	105.9
0.5%NiO/N-TiO ₂	0.77	0.51	0.158	0.3467	10.56	106.6
1.0%NiO/N-TiO ₂	0.77	1.05	0.326	0.3545	11.20	102.3
1.5%NiO/N-TiO ₂	0.77	1.62	0.502	0.3452	10.69	102.7
2.0%NiO/N-TiO ₂	0.77	2.11	0.654	0.3360	11.26	98.4
3.0%NiO/N-TiO ₂	0.77	3.03	0.939	0.3404	10.55	102.8
5.0%NiO/N-TiO ₂	0.77	5.22	1.618	0.2142	13.02	54.1
10.0%NiO/N-TiO ₂	0.77	9.33	2.892	0.2193	12.06	62.4

Table S2. Peak position (eV) of Ti 2p, O 1s, N 1s, and Ni 2p from XPS spectra.

Sample	Binding Energy (eV)							
	Ti 2p _{3/2}	Ti 2p _{1/2}	O 1s	Ni 2p _{3/2}	Ni 2p _{3/2}	N 1s		
TiO ₂	458.92	464.69	530.25	531.95				
N/TiO ₂	458.74	464.54	530.03	531.95			400.0	
0.5%NiO/TiO ₂	458.49	464.22	529.96	531.74	855.40	873.20		
0.25%NiO/N-TiO ₂	458.67	464.43	529.93	531.70			400.6	
0.5%NiO/N-TiO ₂	458.51	464.28	529.76	531.51			401.0	
1.0%NiO/N-TiO ₂	458.54	464.32	529.78	531.53	855.59	873.29	400.0	401.9
3.0%NiO/N-TiO ₂	458.55	464.33	529.90	531.63	855.63	873.30	399.9	401.9
5.0%NiO/N-TiO ₂	458.59	464.35	529.94	531.65	855.71	873.36	399.7	401.9
NiO	-	-	529.42	531.01	854.91	872.60		