

Supporting Information

Solar Light Driven Atomic and Electronic Transformations in Plasmonic Ni@NiO/NiCO₃ Photocatalyst revealed by Ambient Pressure X-ray Photoelectron Spectroscopy

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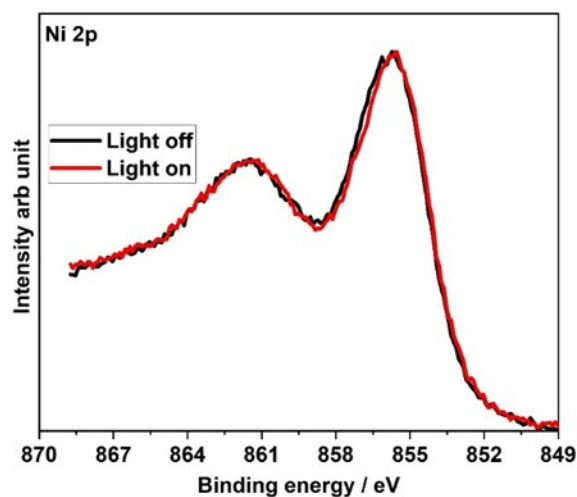


Figure S1: (a) Ni 2p spectra recorded under UHV conditions with light illumination and dark conditions. Spectra of Ni 2p are not significantly affected by light illumination.

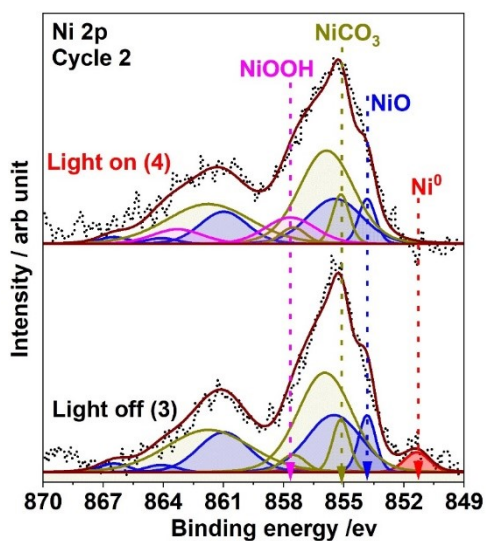


Figure S2:- The second cycle Ni 2p spectrum under dark and light illumination conditions with 1 mbar H₂O is shown in Figure 3. In the main paper, we present the spectra for the first cycle. As can be seen from these spectra, the second cycle is like the first cycle, indicating that Ni 2p is reproducible.

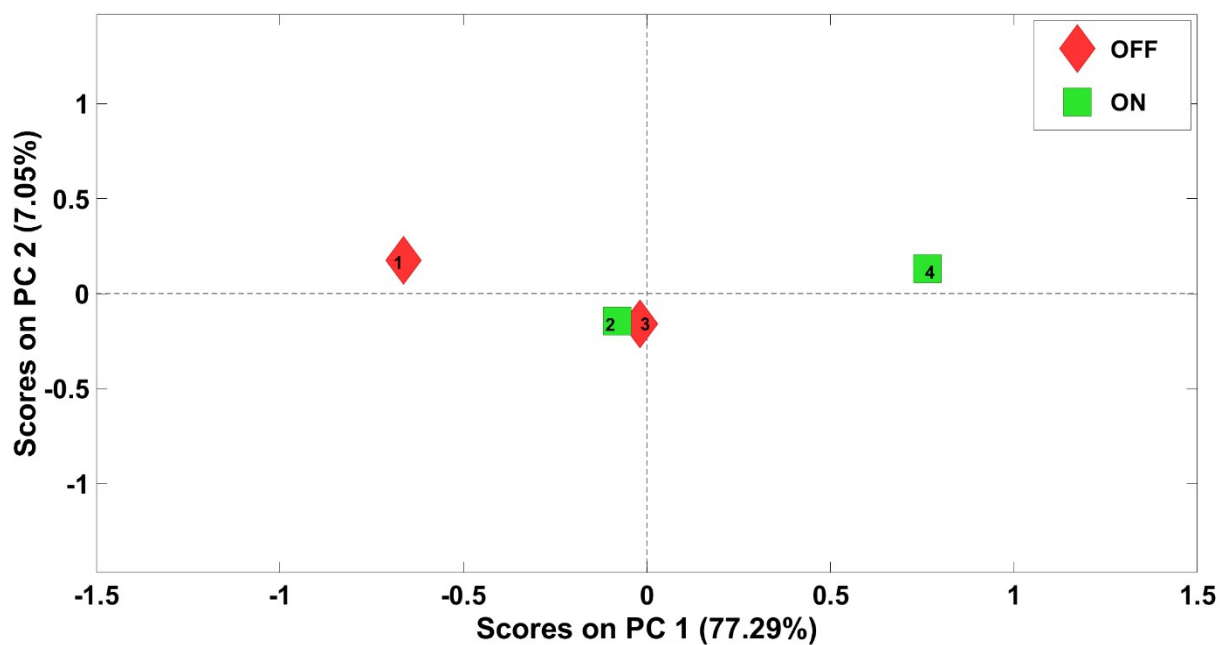


Figure S3: Score plot of the two first PCs on the PCA model of C 1s spectra: red spectra 1 and 3 (light OFF), green samples 2 and 4 (light ON)

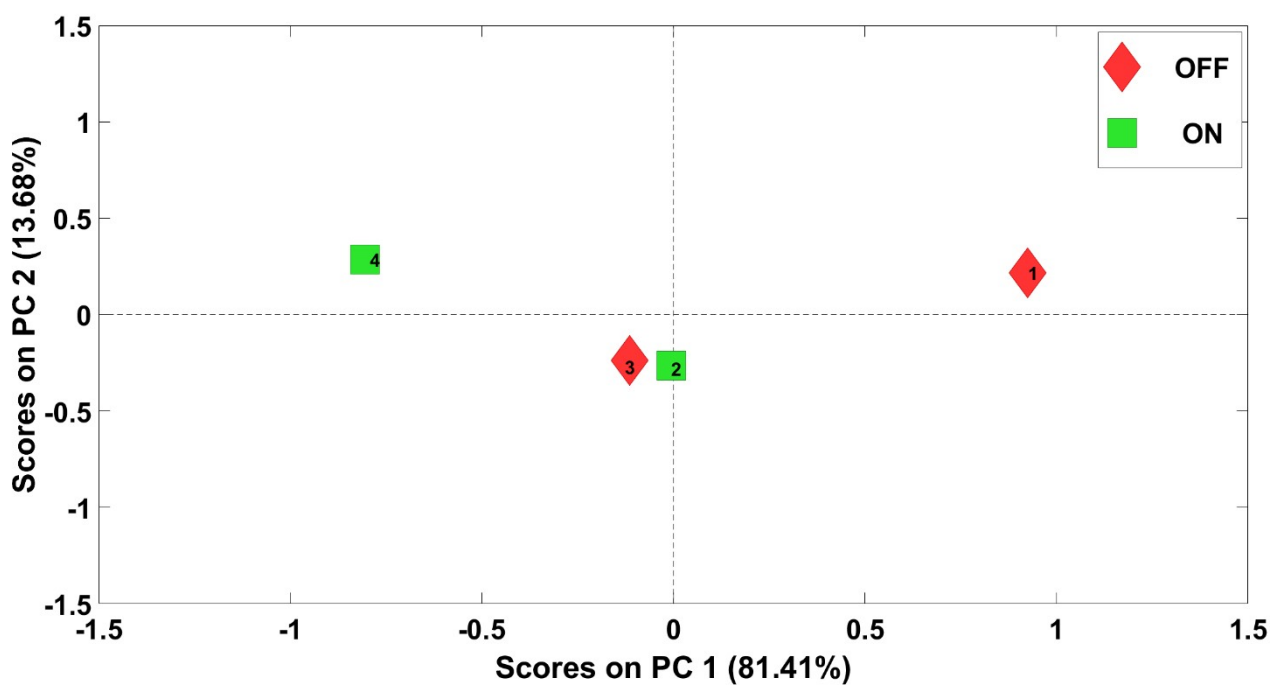


Figure S4: Score plot of the two first PCs on the PCA model of O 1s spectra: red spectra 1 and 3 (light OFF), green samples 2 and 4 (light ON)

Table S1. _ Fitting Parameter for Ni 2p, of Ni@NiO/NiCO₃

Peak no	Ni ⁰			NiO					NiCO ₃					Ni(OOH)	
	1	2	3	1	2	3	4	5	1	2	3	4	5	1	2
Position (eV, UHV)	852.1	855.77	860.12	854.12	855.62	861.06	864.62	866.75	855.20	856.2	858.20	860.50	862.0		
Position (eV, 1 mbar H ₂ O Light OFF)	851.8	855.55	860.2	853.9	855.52	861.02	864.52	866.65	854.8	856.03	858.0	860.26	861.66		
Position (eV, 1 mbar Light H ₂ O ON)				853.9	855.51	860.91	864.51	866.64	854.8	856.09	858.02	860.23	861.72	857.4	864.5
FWHM (eV, UHV)	1.5	2.3	2.2	1.2	3.2	4.2	1.9	2.55	1.26	2.36	1.35	2.15	5.2		
FWHM (eV, 1 mbar H ₂ O Light OFF)	1.5	2.3	1.2	1.2	3.2	4.2	1.9	2.55	1.25	2.36	1.36	2.15	5.2		
FWHM (eV, 1 mbar H ₂ O Light ON)				1.2	3.2	4.2	1.9	2.55	1.25	2.3	1.36	2.15	5.2	3.1	2.79

Table S2. Fitting Parameter for C 1s of Ni@NiO/NiCO₃

	NiO	NiCO₃	-COOH	-C-OH
Position (eV, UHV)	285	288.4		
Position (eV, 1 mbar H₂O Light OFF)	285	288	289.7	286.7
Position (eV, 1 mbar H₂O Light ON)	285	288	289.7	286.7
FWHM (eV, UHV)	2.4	3.5		
FWHM (eV, 1 mbar H₂O Light OFF)	2.2	3.5		
FWHM (eV, 1 mbar H₂O light ON)	2.2	3.5	3.3	2.3

Table S3. Fitting Parameter for O 1s of Ni@NiO/NiCO₃

	NiO	NiCO ₃	-COOH	NiOOH	-C-OH	Ads. H ₂ O	Gas phase peak			
							1	2	3	3
Position (eV, UHV)	530.2	531.5								
Position (eV, 1 mbar H₂O Light OFF)	530.2	531.4				533	534.4	535		
Position (eV, 1 mbar H₂O Light ON)	530.2	531.4	533.2	531.0	531.7	533	534.4	535	534.8	535.4
FWHM (eV, UHV)	2.1	2.4								
FWHM (eV, 1 mbar H₂O Light ON)	1.9	2.1				2	0.83			
FWHM (eV, 1 mbar H₂O light ON)	1.9	2.2	1.95		2.1	2	0.75	0.85		0.1