Supporting Information

Influence of Interface Properties on Charge Density, Band Edge Shifts, and kinetics of Photoelectrochemical Process in p-Type NiO Photocathode

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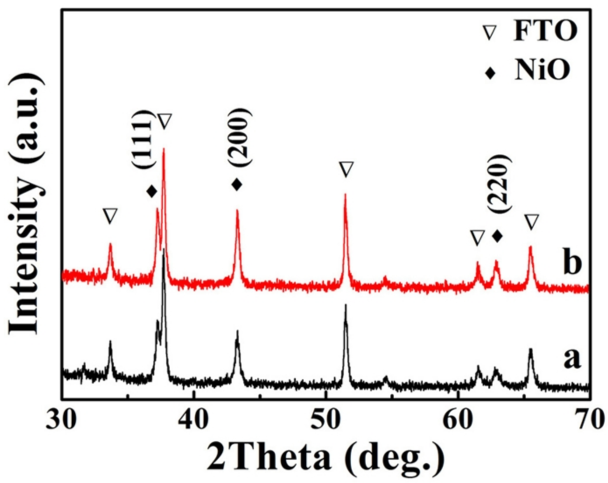

Fig. S1. XRD film diffraction patterns of the (a) NiO and (b) NiO-Ac films. The NiO peaks are indexed according to JCPDF file 65-2901. The FTO peaks are indexed according to JCPDF file 01-077-0447.

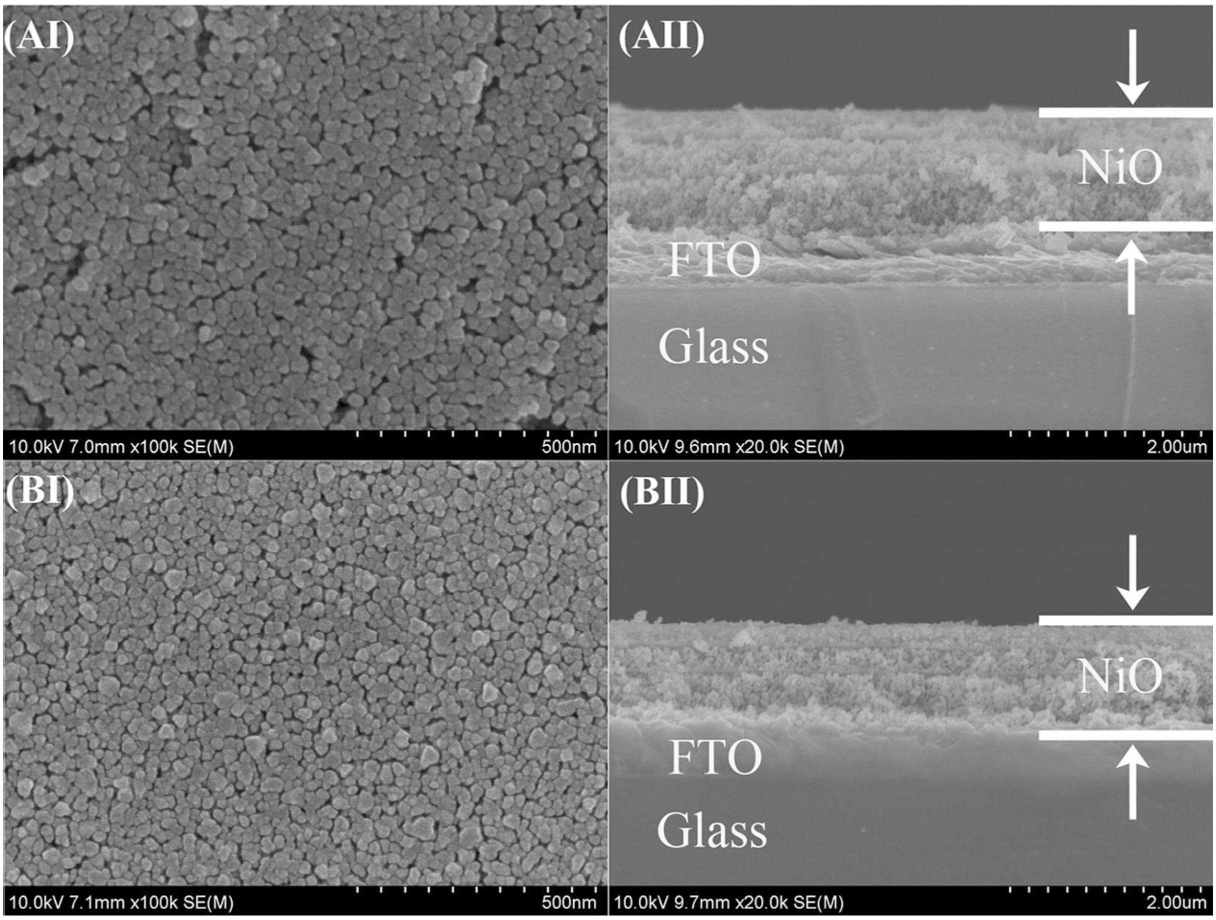

Fig. S2. SEM of (I) surface and (II) cross-section for (A) NiO and (B) NiO-Ac films.

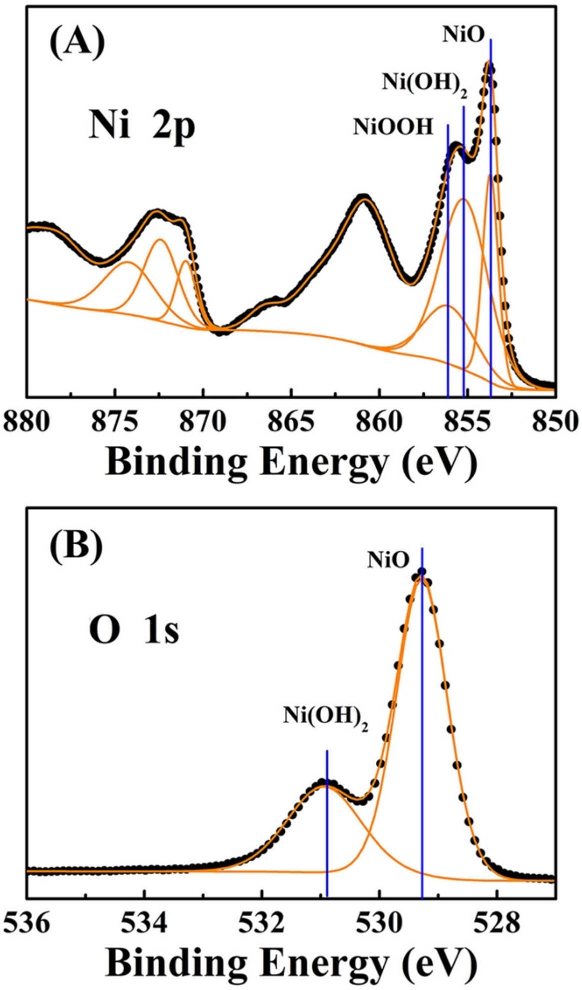

Fig. S3. Results of the XPS analysis: (A) Ni 2p and (B) O 1s spectra for NiO-Ac. Raw data is given by (●) and with fitted components (orange lines).

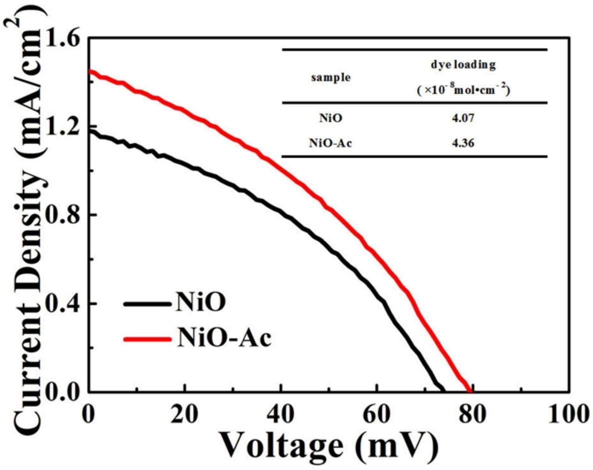

Fig. S4. Current-voltage characteristics of NiO and NiO-Ac devices under standardized AM 1.5 illumination of 100 mW/cm^2 (active area 0.25 cm^2).

Table S1. Comparison of the EIS fitting data for the bare and post-treated NiO DSSCs.

sample	R_s (Ω)	R_{pt} (Ω)	R_t (Ω)	R_{rec} (Ω)	N	C_u [mF/cm^2]	T_{th} [ms]	T_h [s]	L_n [um]	η_{cc}
NiO	10.5	0.75	10.7	280	0.93	0.87	9.3	0.24	5.1	0.96
NiO-S	11.2	1.43	11.9	452	0.93	0.86	10.3	0.39	6.1	0.97
NiO-ozone	10.1	0.46	9.2	200	0.94	0.81	7.4	0.16	4.6	0.95

For a more exact fitting, the capacitance element is replaced by a constant phase element (CPE), in which Y_0(Q) is a constant with the dimension of Siemens·sec$^{\alpha}$, and α(N) is an empirical constant. All the parameters above could achieve by transmission line equivalent circuit. When CPE is in parallel with a resistance, the capacitance can be calculated by the following Equation[1]:

$$C_{\mu} = (QR)^{1/N} / R \quad \text{(S1)}$$

After calculated the parameter C_{μ}, then the other parameters shown in Table S1 were calculated by using the following Equations[2-4]:

$$\tau_h = R_{rec} C_{\mu} \quad \text{(S2)}$$

$$\tau_{th} = R_t C_{\mu} \quad \text{(S3)}$$

$$L_n = d\sqrt{R_{rec} / R_t} \quad \text{(S4)}$$

$$\eta_{cc} = 1 - \tau_{th} / \tau_h \quad \text{(S5)}$$

C_{μ}: Chemical capacitance calculated by fitting data

R_s: Series resistance measured by impedance

R_{pt}: Charge-transfer resistance at counter electrode measured by impedance

R_t: Transport resistance of the film measured by impedance

R_{rec}: Recombination resistance of the film measured by impedance

L_n: hole diffusion length

η_{cc}: charge collection efficiency

All the bias in Fig. 5 have been corrected by Equation:

$$V_{corr} = V_{app} - I_{dark} \cdot (\mathrm{R_s} + (1/3)\,\mathrm{R_t} + \mathrm{R_{pt}}) \quad \text{(S6)}$$

Table S2. Comparison of α parameters calculated from C_μ that obtained by EIS.

sample	α
NiO	0.024
NiO-S	0.023
NiO-ozone	0.053

The parameter α could be achieved by fitting the plots in Fig. 5C using the exponent Equation (3), which represents for the depth of the trap energy distribution, and the α is an absolute value.

Table S3. Comparison of short-circuit photocurrent density (J_{sc}), open-circuit photovoltage (V_{oc}), fill factor (FF), measured under AM 1.5, of p-type DSSCs employing bare NiO and post-treated NiO film.

sample	V_{oc} [mV]	J_{sc} [mA/cm^2]	FF [%]	η [%]
NiO	74	1.18	37.7	0.032 ± 0.002
NiO-S	81	1.13	39.2	0.036 ± 0.002
NiO-ozone	66	0.72	42.2	0.020 ± 0.001
NiO-Ac	80	1.45	36.2	0.042 ± 0.002

Table S4. Surface analysis by XPS spectra for the $Ni(CH_3COOH)_2$ treated NiO.

sample	O1s			$Ni2p_{3/2}$			(NiO:$Ni(OH)_2$:NiOOH)
	NiO [eV]	$Ni(OH)_2$ [eV]	NiOOH [eV]	NiO [eV]	$Ni(OH)_2$ [eV]	NiOOH [eV]	
NiO-Ac	529.28	530.94	-	853.71	855.20	856.05	1:2.49:0.90

Notes and References

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