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

Supporting Information

Surface Treatment of ZnO Film by Carbon Nanotubes for Efficient and Stable Perovskite Solar Cells

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Figure 1 reveals the X-ray pattern of pure CNTs. As shown, a diffraction peak located at $2\theta = 26.1^{o}$ attributed to (002) crystal facet. Additionally, other two weak peaks at 42.8^{o} and 44.7^{o} related to (100) and (101) crystal facets, respectively. This pattern of CNT matched well with standard graphitic phase (JCPDS: 01–0646) [1]. The FTIR spectrum of CNTs was recorded at room temperature as shown in Figure S1b. The peak at the wavenumber of 1608 cm^{-1} is corresponded to the C=C stretching vibration of carbon backbone in the CNT structure [2]. The FTIR bands at 1073 cm^{-1} and 3345 cm^{-1} are assigned to the carbonyl (C-O) and hydroxyl (O–H) acid groups, respectively, indicating decorating CNTs with oxygenated functionalities after acid oxidation [3]. Besides, the C–H symmetric and asymmetric stretching vibrations are centered at wavenumbers of 2921 cm^{-1} and 2854 cm^{-1}, respectively [4]. The UV–vis absorption spectrum of CNTs suspended in water (Figure S1c) shows a strong absorption peak at 265 nm, which corresponds to an electronic transition ascribed of π–π * transition within the sp^2-localized carbon atoms [5]. As shown in Figure S1d, TEM image of CNT drop-cast on a glass substrate demonstrates that pure CNTs appeared with long tube morphology and possess an entangled geometry, which further reveals the CNTs are one-dimensional nanostructured material. Clearly, from above findings, it can be confirmed that the desired CNTs have been successfully synthesized.

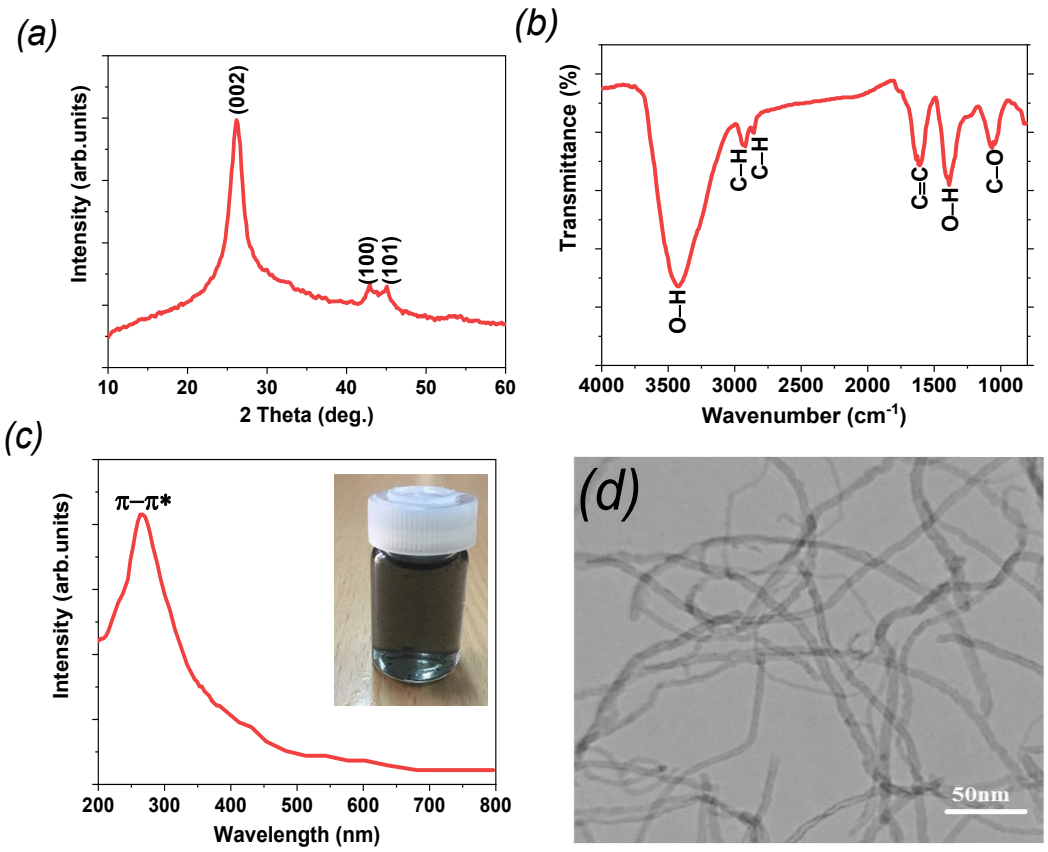

Figure S1. (a) XRD pattern of CNT. (b) FTIR spectrum of CNT. (c) UV-vis absorption spectrum of CNT. Inset: the photograph of CNT suspension. (d) TEM image of CNT.

Table S1. J-V curves in reverse and forward scans of best-performing PSCs with and without CNT.

Device	V_{oc}[a] (V)	J_{sc}[b] (mA/cm^2)	FF[c] (%)	PCE[d] (%)	HI (%)
Reverse (Ref.)	0.98	20.48	75	15.05	10.5
Forward (Ref.)	0.95	19.42	73	13.47	
Reverse (2%)	1.06	22.61	80	18.79	1.6
Forward (2%)	1.058	22.41	78	18.49	

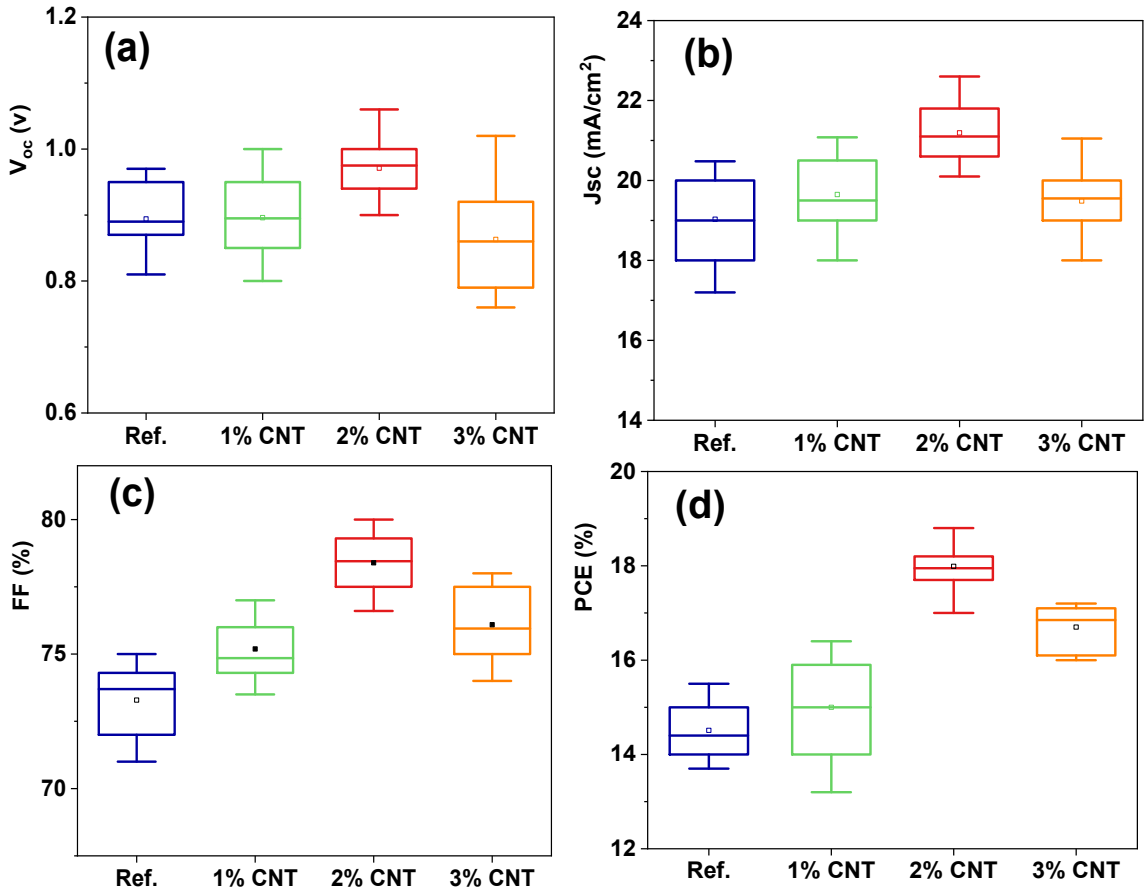

Figure S2. Device statistics of V_{OC}, J_{SC}, FF, and PCE of PSCs using ETL incorporated with or without CNT modification. Every box shows the parameter distribution of 20 devices.

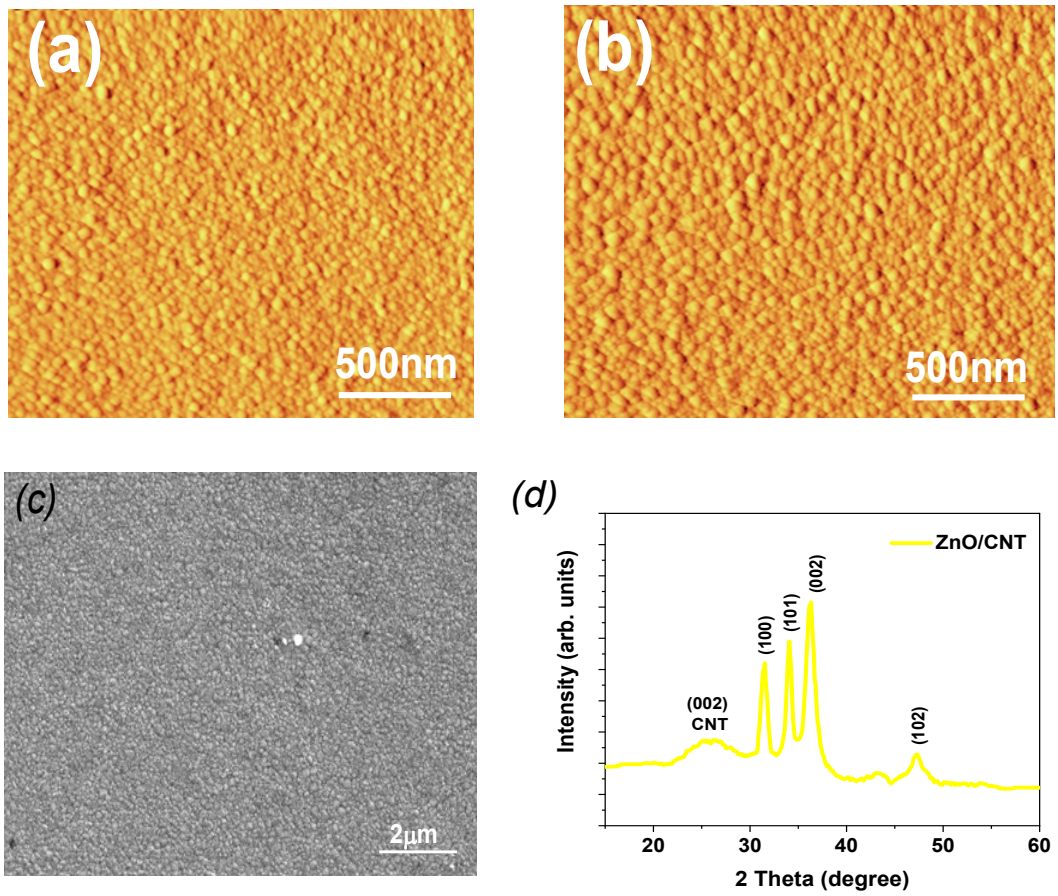

Figure S3. a) AFM image of pure ZnO. b) AFM image of ZnO-containing 2% CNT. c) SEM image of ZnO/CNT film. d) XRD pattern of ZnO/CNT film.

Table S2. Sumarized parametrs obtained from EIS analysis.

Sample	Z_1' [Ω]	$Z'_{2\,[\Omega]}$
ZnO/PVK	2.9	26.2
ZnO:CNT/PVK	1.6	23.4

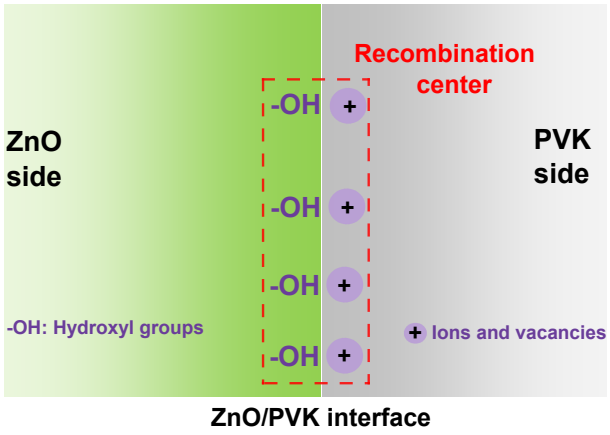

Figure S4. Illustration showing the positive ion localization caused by the surface-negative charges (–OH) of ZnO.

References

[1] M. K. A. Mohammed, A. K. Al-Mousoi, H. A. Khalaf , *Optik* **2016**, *127*, 9848–9852.

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[3] M. K. A. Mohammed, *Optik* **2020**, *223*, 165607.

[4] D. S. Ahmed, M. R. Mohammad, M. K. A. Mohammed, *Nanosci. Nanotechnol.-Asia* **2020**, *10*, 127−133.