Supporting Information

Application of NADH- modified ZnO electron transport layer in high performance organic solar cells

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Experimental details

Material: PM6, Y6 and L8-BO were purchased from Organtec. Ltd. All solvents were purchased from Sigma. NADH powder purchased from McLean. The ITO came from Wuhu Jinghui Electronic Technology Co., Ltd; The Ag pellets were from Tim New Material Technology Co., Ltd.

Preparation of Material: A certain amount of NADH powder is dissolved in the ZnO precursor solution.The active layer (PM6:Y6, PM6:L8-BO) was maintained at a ratio of 1.0:1.2 (w/w), dissolved with a total concentration of 16 mg/mL chloroform and 0.5% 1-chloronaphthalene and 0.25% DIO, respectively, and stirred at 50℃ for 2 hours.

Device preparation: All OSCs were prepared using ITO/ETL (ZnO or ZnO:NADH)/ PM6:Y6 /MoO_3 /Ag conventional structure. The resistance of ITO substrate was about 10 Ω sq^{-1}. First, ITO was ultrasonic cleaned in detergent for 20 min to remove surface stains, followed by ultrasonic cleaned in deionized water, acetone, isopropyl alcohol and anhydrous ethanol for 20 min to remove surface organic residues. Then the cleaned ITO was put into the drying box of 80℃ and dried for more than 12 hours for reserve. The dried ITO sheet was put into the plasma machine and treated with oxygen plasma gas for 10 min to reduce its surface roughness. The ZnO and ZnO:NADH was filtered and then coated on the surface of ITO with 40 s rotation at 4000 rmp/min, and then heated on the heating table at 200 ℃ for 60 min. After that, the PM6:Y6 and PM6:L8-BO were applied to the ETL-coated ITO in a 30 s rotation at 3000 rpm/min and 3000 rpm/min, respectively. ITO/ETL/active layer was heated on a 110 ℃ and 100 ℃ respectively for 7 ~ 10 min to form an active layer about 100 nm thick. After that, Finally, 2 nm of MoO_3 and 100 nm of Ag were steam-plated on the ITO/HTL//active layer surface in turn at 2.8 x 10^{-4} Pa.

Equipment description: The X-ray diffraction curve (XRD) of $ZrSe_2$ was determined by Brooke Advanced diffractometer. An atomic force microscope (AFM) was

photographed using the NanoScope NS3A system (Bruker, DEU). X-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS) were performed on the Thermo Scientific Escalab 250Xi instrument equipped with Mg-Kα source. The $J-V$ curves of all devices were measured using a Keithley 2400 source meter (AM 1.5G). EQE spectra were determined using the SRF50 system. The photoluminescence spectra were measured by SPEX 1681 automatic fluorescence spectrometer. Contact Angle was measured by static propulsive contact. The UV-VIS transmission spectrum of ETL was studied by HP8453 UV-VIS spectrophotometer. The electrochemical impedance spectra (EIS) were obtained using a Zennium-IM6 electrochemical workstation under dark conditions.

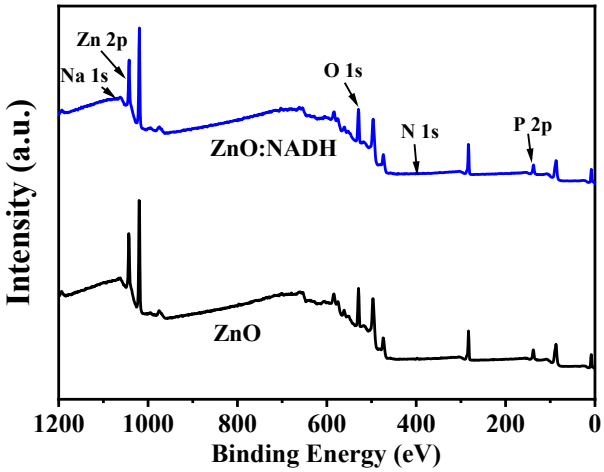

Figure S1. Full-scan XPS spectra of ZnO and ZnO: NADH.

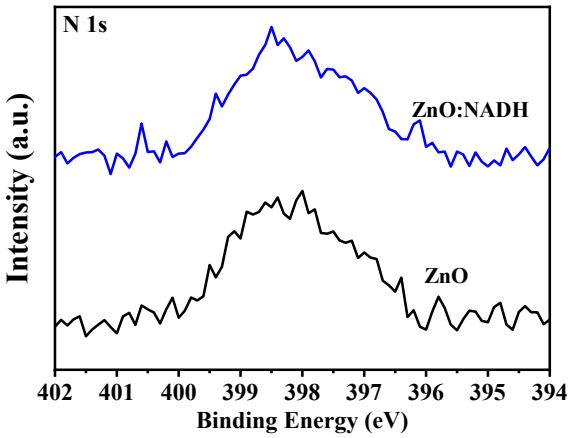

Figure S2. N 1s XPS of ZnO and ZnO: NADH.

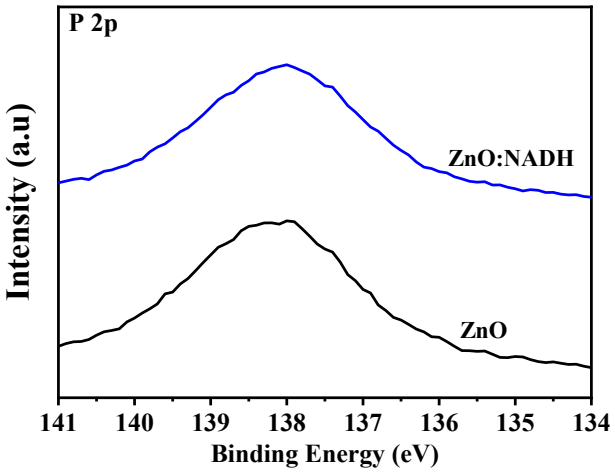

Figure S3. P 2p XPS of ZnO and ZnO: NADH.

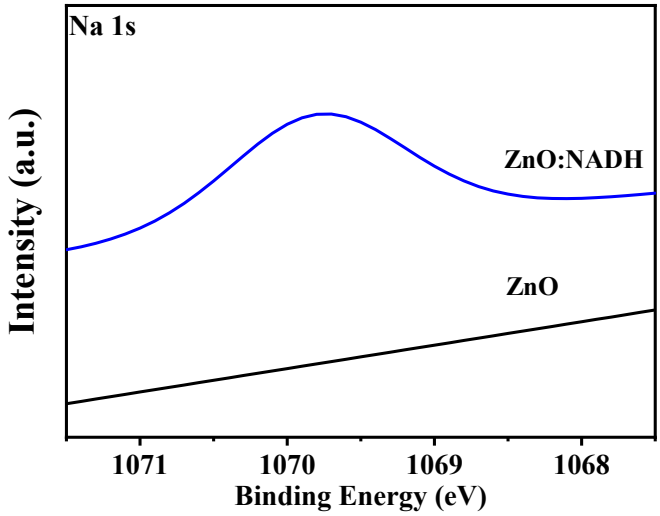

Figure S4. Na 1s XPS of ZnO and ZnO: NADH.

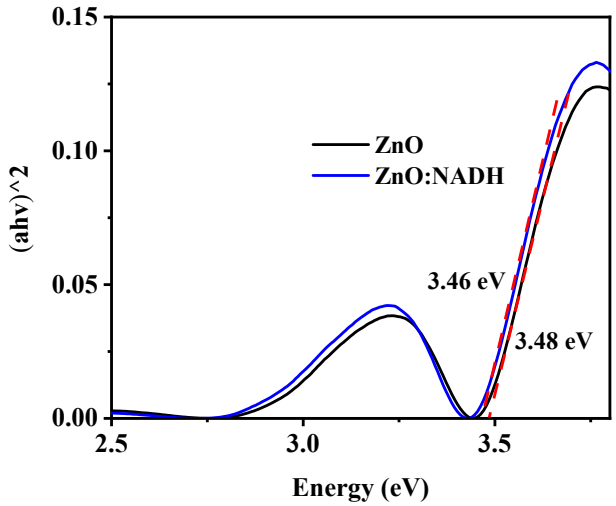

Figure S5. UV of ZnO and ZnO:NADH.

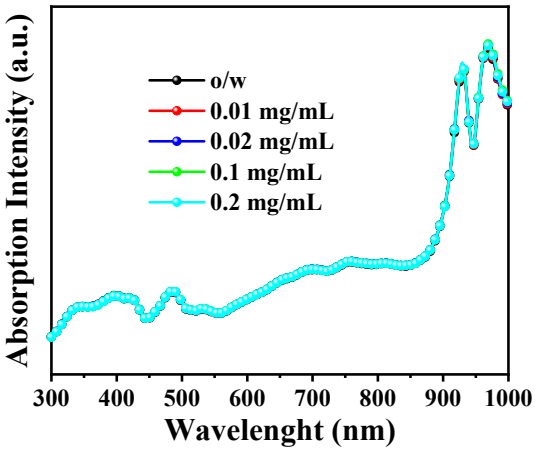

Figure S6. Absorption spectra of ITO/ZnO and ITO/ZnO:NADH.

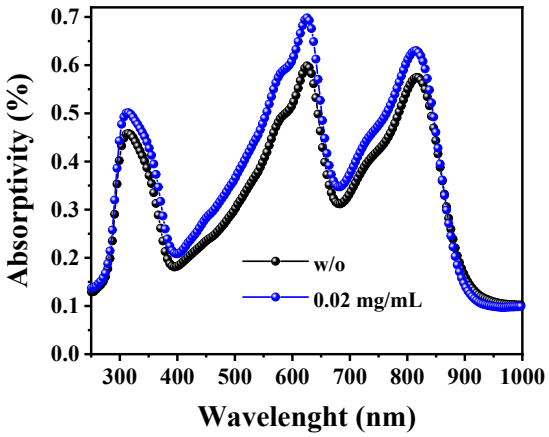

Figure S7. Absorption spectra of ITO/ZnO/PM6:Y6 and ITO/ZnO:NADH/ PM6:Y6.

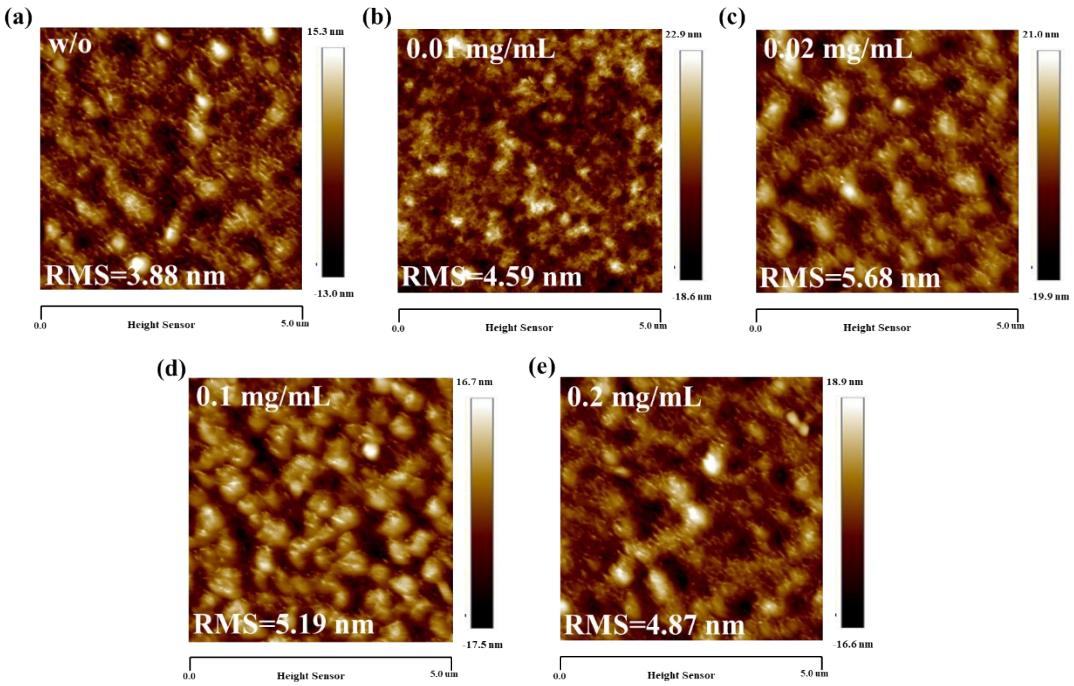

Figure S8. AFM of ITO/ZnO/PM6:Y6 and ITO/ZnO:NADH/PM6:Y6.

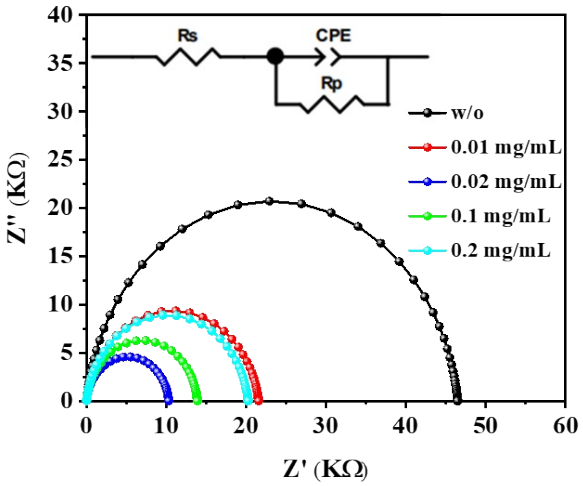

Figure S9. Electrochemical impedance spectroscopy (EIS) of ZnO and ZnO:NADH.

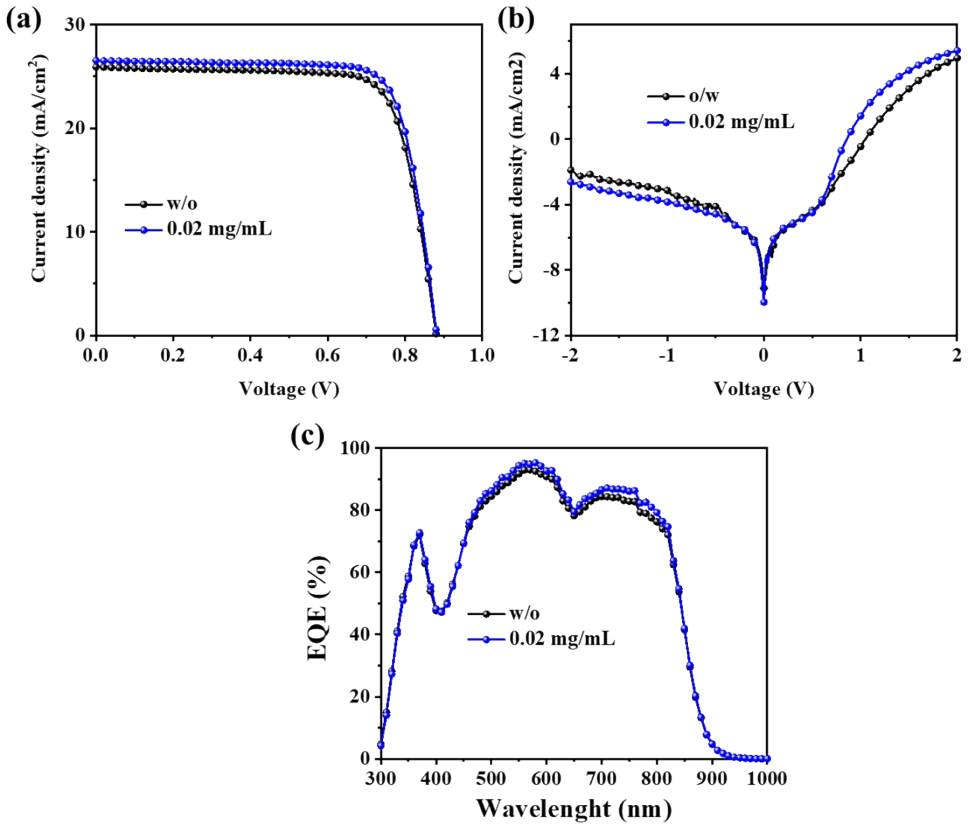

Figure S10. (a) *J-V* curves, (b) dark *J-V* curves, (c) external quantum efficiency (EQE) spectra of OSCs with PM6:L8-BO as active layer.

Table S1. Content proportion of each elements.

	O (area/wt %)	**Zn (area/wt %)**	**N (area/wt %)**	**P (area/wt %)**	**Na (area/wt %)**
ZnO	149,071.3 (17.81%)	642,363.6 (76.77%)	3514.2 (0.42%)	40319.0 (4.82%)	0 (0%)
ZnO:NADH	143,658.7 (20.18%)	525,913.7 (73.91%)	3381.2 (0.47%)	36189.4 (5.08%)	2455.7 (0.34%)

Table S2. The proportion of each component in O 1s.

Type	Lattice oxygen	Defective oxygen	Zn-OH	C-OH
ZnO	0.33	0.46	0.20	0
ZnO:NADH	0.35	0.30	0.23	0.11

Table S3. Electrical Conductivity of the device (ITO/ETL/Ag).

Type	**σ（μS/cm）**
w/o	1.14
0.02 mg/mL	3.27

Table S4. EIS test results of the equipment.

Type	R_s (Ω)	R_{bulk} (kΩ)
w/o	45.48	46.42
0.01 mg/mL	45.26	21.55
0.02 mg/mL	33.44	10.29
0.1 mg/mL	34.95	13.87
0.2 mg/mL	43.24	20.22