

Supporting Information for

Facile Approach to Preparing a Vanadium Oxide Hydrate Layer as a Hole-Transport Layer for High-Performance Polymer Solar Cells

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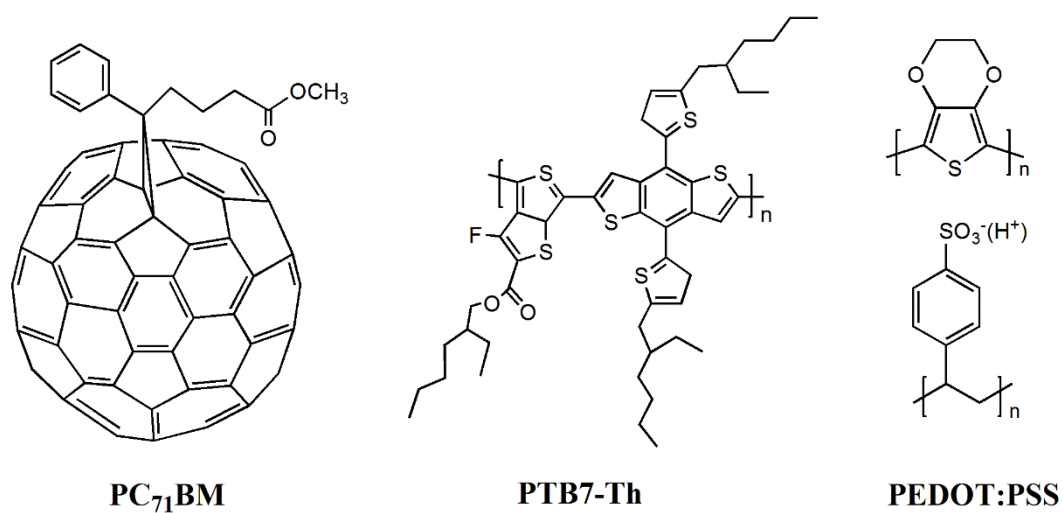


Figure S1. Schematic molecule structures of PC₇₁BM, PTB7-Th, PEDOT:PSS.

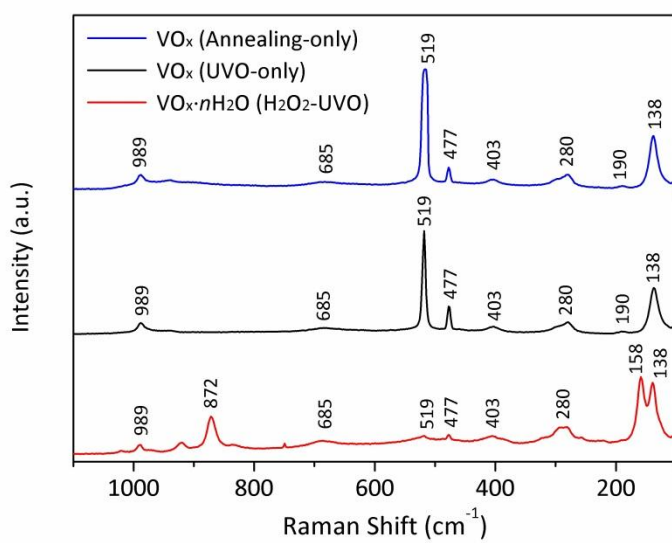


Figure S2. Micro-Raman spectra of the as-prepared VO_x·*n*H₂O (H₂O₂-UVO) and VO_x layers.

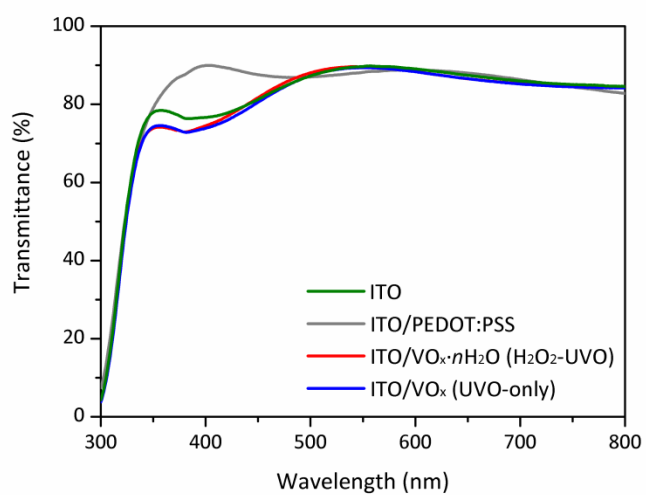


Figure S3. Optical transmittance spectra of the bare ITO, PEDOT:PSS and $\text{VO}_x \cdot n\text{H}_2\text{O}$ (H_2O_2 -UVO) and VO_x (UVO-only) layers.

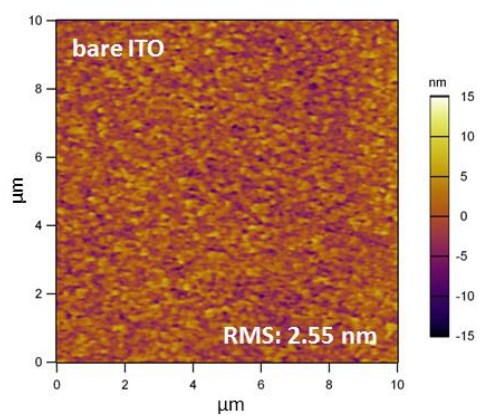


Figure S4. AFM height image of the bare ITO. The scan size is $10\ \mu\text{m} \times 10\ \mu\text{m}$.

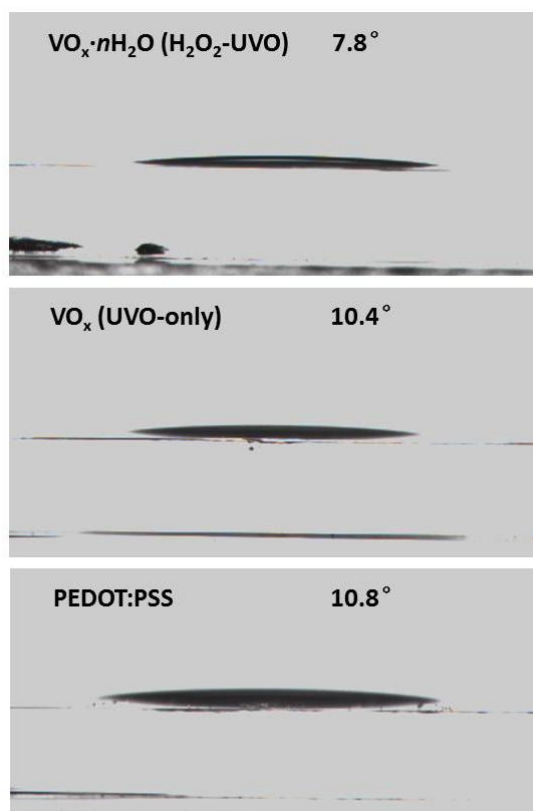


Figure S5 Measured contact angle between a drop of 1,2-dichlorobenzene and the HTL. VO_x·*n*H₂O (H₂O₂-UVO), VO_x (UVO-only), and PEDOT:PSS layers from top to bottom, respectively.

Table S1. Device performance of the PSCs (based on PTB7-th:PC₇₁BM) with VO_x *n*H₂O (H₂O₂-UVO) layer with varied concentration.

precursor	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	PCE (%)
1.0 mg/mL	0.796	16.49	68.2	8.11
1.5 mg/mL	0.790	14.69	63.6	7.38
2.0 mg/mL	0.772	15.15	61.4	7.18

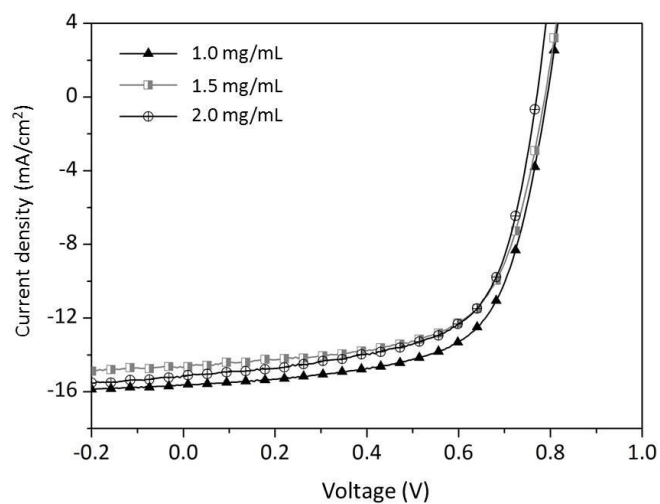


Figure S6. J – V curves of the PSCs (based on PTB7-th:PC₇₁BM) with VO_x *n*H₂O (H₂O₂-UVO) layer with varied concentration under 1 sun illumination condition.

Table S2. Device performance of the PSCs based on P3HT:PC₆₁BM with different HTLs.^a

device	hole transport layer	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	PCE (%) ^b
A'	PEDOT:PSS	0.647	7.90	62.26	3.18(3.32)
B'	VO _x ·nH ₂ O (H ₂ O ₂ -UVO)	0.638	8.12	62.24	3.24(3.32)
C'	VO _x (UVO-only)	0.630	7.75	60.98	2.98(3.04)
D'	VO _x (annealing-only)	0.637	8.14	52.38	2.72(2.90)

^aStatistical data achieved from 10 independent devices. ^bThe maxima PCEs are in the brackets.

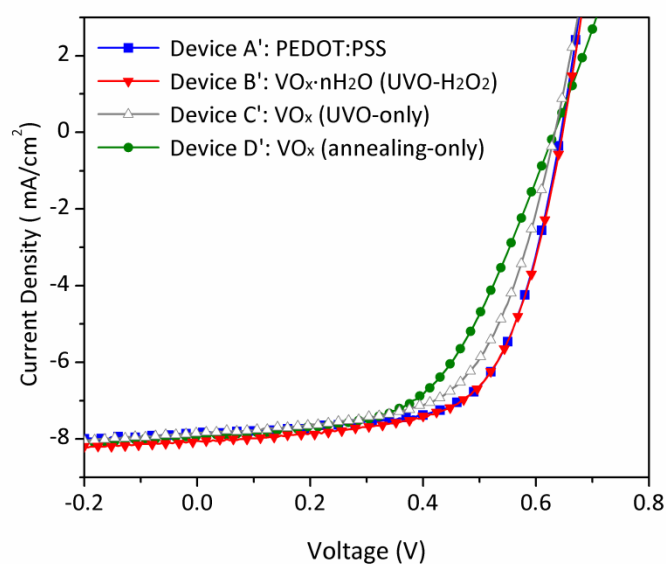


Figure S7. J – V curves of best performing devices based on P3HT:PC₇₁BM with different HTLs under 1 sun illumination condition.

Space charge limited current (SCLC) measurements

The SCLC devices or hole-only devices were fabricated with a configuration of ITO/HTL/PTB7-th:PC₇₁BM/MoO₃/Ag. The SCLC can be written as $J_{SCLC} = 9\epsilon_0\epsilon_r\mu_h(V-V_{BI})^2/(8L^3)$: where J is current density, ϵ_r is dielectric constant of the fullerene derivatives (normally a value of 3 is used), ϵ_0 ($8.8541878176 \times 10^{-12}$ F/m) is the permittivity of vacuum, μ_h is hole carrier mobility, L is film thickness, $V = V_{appl} - V_{bi}$, V_{appl} is the applied potential, and V_{bi} is the built-in potential resulting from work function difference between two electrodes (in this device, $V_{bi} = 0.6$ V)¹. To evaluate the μ_h value, the log J - V line obtained in dark was fitted using a function of $y = a + 2x$ and electron mobility (μ_h) was calculated from the y-intercept of the fitting line.

Reference.

1. Morsli1, M.; Cattin, L.; Bernède, J. C.; Kumar, P.; Chand, S. J - V Characteristics of Dark and Illuminated Classical and Inverted Organic Solar Cells Based on the CuPc/C₆₀ Heterojunction. *J. Phys. D: Appl. Phys.* **2010**, *43*, 335103.