

Suppression of SAM desorption by engineering polyoxometalate interface for inverted perovskite solar cells

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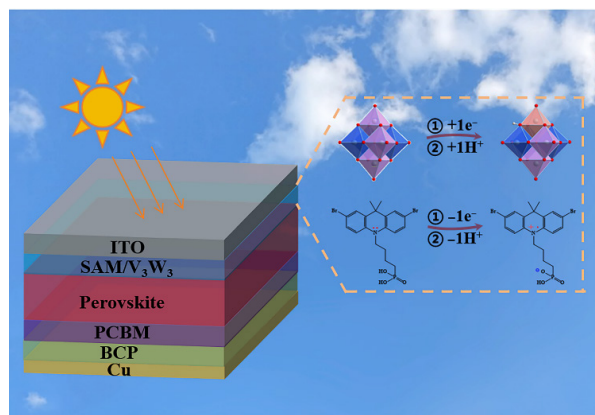
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ABSTRACT: Self-assembled monolayers (SAMs) have markedly enhanced the power conversion efficiency (PCE) of inverted perovskite solar cells (PSCs); however, the desorption of SAMs limits the long-term stability of the devices. Herein, Lindqvist-type polyoxometalates (POMs) $[V_nW_{6-n}O_{19}]^{(n+2)-}$ ($n = 1-3$) were incorporated into SAMs. By leveraging vanadium to establish V(V)/V(IV) redox couples, the electron cloud density of the V–O–W bridging oxygens was significantly enhanced, promoting tridentate anchoring between the SAMs and indium tin oxide via proton-coupled electron transfer (PCET). This increased the anchoring ratio from 29.93% to 53.98% while reducing the desorption rate from 30.7% to 5.6%. The robustly anchored SAMs facilitate the crystallization of high-quality perovskites and effectively suppress interfacial defects, significantly improving the hole-extraction efficiency and increasing the PCE from 23.68% to 25.15% under continuous AM 1.5 G illumination. Moreover, the device stability was markedly enhanced, with the target retaining 90.7% of its initial efficiency after 1200 h of continuous maximum power point tracking (compared to 53.8% for the control). This study demonstrates that POMs can effectively suppress the desorption of SAMs and reduce interfacial losses, offering new insights for fabricating highly efficient and stable PSCs.

KEYWORDS: polyoxometalates, perovskite solar cells, self-assembled monolayers, proton-electron coupled transfer, buried interface



1 Introduction

Inverted perovskite solar cells (PSCs) with the p-i-n configuration exhibit remarkable power conversion efficiencies (PCEs), with certified values currently exceeding 27%. Consequently, this architecture merits further in-depth investigation for advancing the commercialization of PSCs [1–4]. The rapid gain in the PCE of PSCs is primarily attributed to the use of self-assembled molecules (SAMs) as hole transport layers (HTLs) [5–7]. SAMs are typically composed of three components: an anchoring group, a linker, and a functional group, which play a pivotal role in mitigating charge-transport losses [8–11]. SAMs employing phosphonic acids (PAs) as the anchoring group have found the most widespread

application [12, 13]. Despite these advantages, a considerable proportion of SAMs are anchored onto the surface of indium tin oxide (ITO) via monodentate or bidentate coordination, failing to form the most robust tridentate anchoring configuration [14, 15]. However, during spin-coating of the perovskite precursor (PVK), polar solvents such as *N,N*-dimethylformamide (DMF) and dimethyl sulfoxide (DMSO) are inevitably introduced. In this process, weakly bound PA groups tend to detach, creating interfacial defects and compromising the crystallization quality [16–19]. Researchers have proposed various strategies for optimizing the HTL/PVK interface. For example, Chang et al. introduced an n-HfO_x layer, rich in hydroxyl and Lewis acid groups, at the NiO_x/SAM interface to promote tridentate PA coordination, thereby enhancing the stability of the SAM [20]. Wang et al. reported sulfadiazine (SDZ)-induced proton abstraction from the PA functionalities in SAMs, reinforcing the electrostatic anchoring. This modification of the HTL layer improved the crystallinity of PVK and enhanced the effective charge extraction [21]. Therefore, identifying suitable materials to optimize the HTL/PVK interface is an important route for improving the performance and stability of PSCs.

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Polyoxometalates (POMs) are a unique class of nanoscale metal-oxide clusters composed of early transition metals (typically Mo, W, V, Nb, and Ta) bridged by shared oxygen atoms [22–40]. As interfacial modifiers, they offer a threefold advantage. First, by tuning the ratio of metal ions, the redox activity can be optimized, thereby promoting oxidation of the HTL materials to generate radical cations, consequently enhancing the hole-transfer efficiency. Second, their energy levels are aligned with those of SAMs, promoting hole extraction and transfer while reducing interfacial energy losses. Third, their abundant oxygen-rich sites can effectively passivate defects in the PVK and enhance its crystallinity. Owing to these advantages, POMs have been widely used in optimizing HTL/PVK interfaces. Yang et al. used $[\text{Cu}_2(\text{BTC})_{4/3}(\text{H}_2\text{O})_2]_6$ $[\text{H}_3\text{P}(\text{Mo}_{12}\text{O}_{40})_2]$ (POM@Cu-BTC) to achieve controlled oxidation of spiro-OMeTAD, significantly enhancing the hole mobility of the HTL, while the optimized highest occupied molecular orbital (HOMO) level alignment further facilitated efficient hole transfer [41]. Huang et al. functionalized the cationic components of POMs with ammonium groups, constructing a stable HTL/PVK interlayer that enabled defect passivation and effectively stabilized the $[\text{PbI}_6]^{4-}$ octahedra [42]. Beyond the HTL/PVK interface, our prior research revealed that incorporating POMs into the PVK precursor can passivate grain-boundary defects and promote crystal growth [43–45]. By tuning the redox capability of POMs, Pb^0 can be effectively oxidized to Pb^{2+} , whereas I^0 can be reduced to I^- [46]. Furthermore, POMs with appropriately matched energy levels achieved favorable alignment with both SnO_2 and PVK, significantly improving the carrier-transport efficiency [47].

Electron acceptance reduces the metal centers in POMs, a process coupled to concurrent protonation at neighboring oxygen sites via the proton-coupled electron transfer mechanism. Such synergy effectively stabilizes the reduced state by mitigating excessive charge accumulation. Matson et al. demonstrated ineffective coupling of reduction and protonation in Lindqvist-type polytungstate (W_6), whereas VW_5 , formed upon vanadium substitution at the tungsten sites, exhibits proton-coupled electron transfer (PCET) activity. This is attributed to the significantly lower empty d-orbital energy of vanadium compared to tungsten, which not only provides the $\text{V(V)}/\text{V(IV)}$ redox couple but also enhances the basicity of the V-O-W bridging oxygen sites, thereby promoting hydrogen atom uptake [48]. On this basis, we selected the $[\text{V}_n\text{W}_{6-n}\text{O}_{19}]^{(n-2)-}$ ($n = 1-3$) series of POMs as post-treatment agents for SAMs. Upon reduction, the vanadium centers in the POMs accept electrons, with concomitant proton binding. This exposes electron-rich oxygen atoms on the PA groups and promotes the formation of $\text{O}\cdots\text{O-H}$ hydrogen bonds with hydroxyl groups on the surface of ITO, enhancing the binding strength between the SAM and ITO. Among this series, V_3W_3 has the most

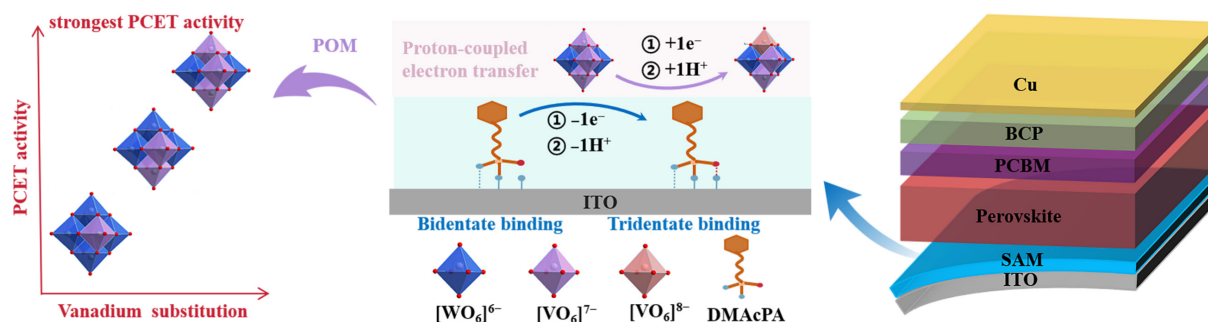
vanadium sites, resulting in the strongest PCET activity (Scheme 1). X-ray photoelectron spectroscopy (XPS) confirmed that post-treatment V_3W_3 increased the tridentate anchoring ratio of the SAM from 29.93% to 53.98% and decreased the desorption rate from 30.7% to 5.6% after rinsing with dimethyl formamide. In addition, ultraviolet photoelectron spectroscopy (UPS) and Kelvin probe force microscopy (KPFM) revealed that V_3W_3 modification increased the work function of the SAM, optimizing the energy-level alignment at the HTL/PVK interface and facilitating efficient hole transfer. Consequently, the optimal device achieved a PCE of 25.15%, with 90.7% preservation of its original PCE following 1200 h of continuous maximum power point tracking (MPPT) under AM 1.5 G irradiation under nitrogen. This study provides new insights for constructing high-efficiency, stable PSCs through POM modulation of the HTL/PVK interface.

2 Results and discussion

2.1 Synthesis and characterization of POMs

Lindqvist-type $\text{K}_3\text{VW}_5\text{O}_{19}$ (VW_5), $\text{K}_4\text{V}_2\text{W}_4\text{O}_{19}$ (V_2W_4), and $\text{K}_5\text{V}_3\text{W}_3\text{O}_{19}$ (V_3W_3) were synthesized using literature methods [49, 50]. The structures and electrospray ionization–mass spectrometry (ESI–MS) profiles of these materials are presented in Figs. 1(a)–1(c). The m/z values of 637.75, 1144.14, and 563.01 correspond to $\text{HVW}_5\text{O}_{19}^{2-}$, $\text{H}_3\text{V}_2\text{W}_4\text{O}_{19}^{3-}$, and $\text{K}_3\text{V}_3\text{W}_3\text{O}_{19}^{2-}$, respectively. The corresponding Fourier-transform infrared (FTIR) spectra [51] and transmission electron microscopy images [52] are presented in Figs. S1 and S2 in the Electronic Supplementary Material (ESM), respectively. Energy-dispersive spectroscopy elemental mapping (Fig. S2 in the ESM) and XPS (Figs. S3–S5 in the ESM) revealed a highly uniform distribution of V, W, O, and K. The results collectively confirm the successful synthesis of VW_5 , V_2W_4 , and V_3W_3 . The three POMs were individually spin-coated onto the SAM and analyzed using FTIR (Fig. 1(d)). Attenuation of the P-O-H peak signal, coupled with the relative enhancement of the P=O signal upon incorporating the POMs, demonstrates that the POMs effectively deprotonate the PA groups, thereby reinforcing the anchoring effect.

To determine the energy levels of the POMs, cyclic voltammetry curves of VW_5 , V_2W_4 , and V_3W_3 were constructed from the data obtained using an Ag/AgCl reference electrode. The corresponding first oxidation peak potentials were 0.28, 0.41, and 0.61 V, respectively (Fig. S6 in the ESM). According to the equation $E_{\text{vacuum}} = -E_{\text{Ag}/\text{AgCl}} - 4.72$ V, the corresponding energy levels of the HOMO relative to the vacuum level were calculated to be -5.00 , -5.13 , and -5.33 eV, respectively. Furthermore, using this data combined with ultraviolet–visible (UV–vis) spectroscopy (Fig. 1(e))



Scheme 1 POMs promote the transformation of SAM into tridentate anchoring via the PCET, enhancing the stability of SAM.

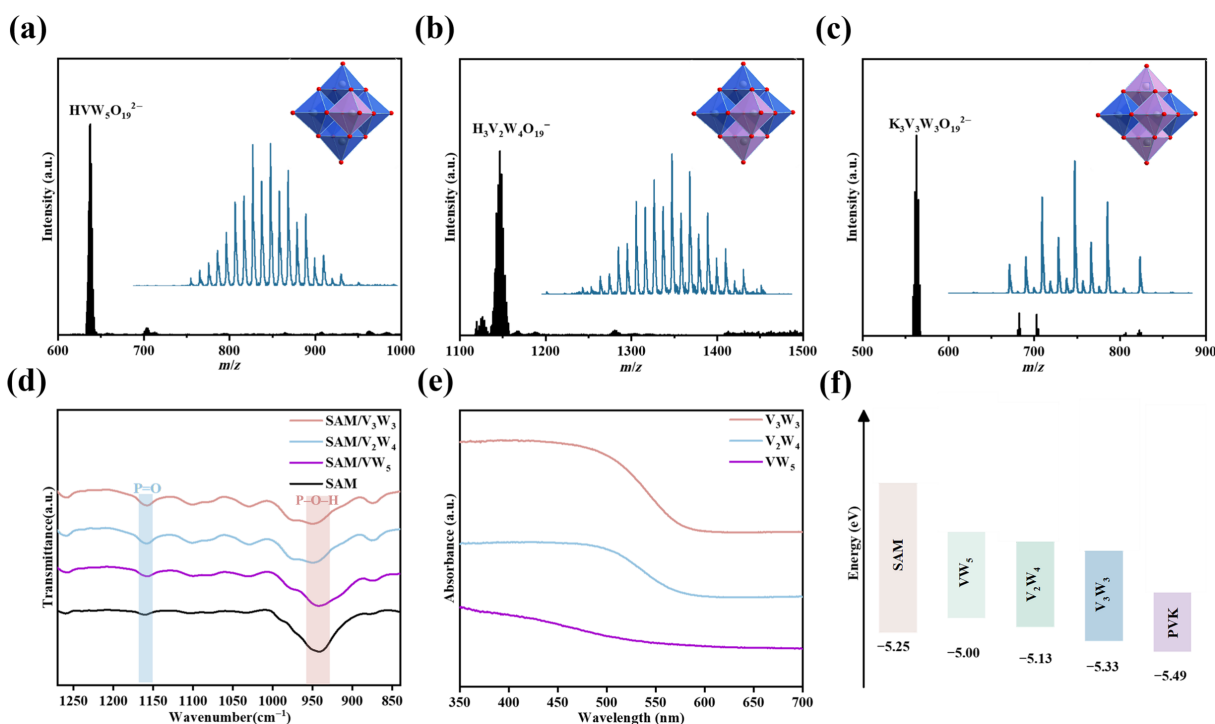


Figure 1 ESI-MS spectra corresponding to (a) VW_5 , (b) V_2W_4 , and (c) V_3W_3 . (d) IR spectra of three POMs incorporation into SAM. (e) UV-vis spectra and (f) energy level diagram of the three POMs.

and Figs. S7–S9 in the ESM), an energy-level diagram of the SAM/POMs/PVK integrated system was constructed (Fig. 1(f)). The HOMO energy level of V_3W_3 exhibits more favorable alignment with PVK and the SAM. This optimized energy level alignment ensures more efficient hole transfer.

2.2 Mechanism of proton-coupled electron transfer at HTL/PVK interface

Previous studies have shown that owing to intrinsic differences in the energy levels of the V 3d and W 5d orbitals, the V(V)/V(IV) couple is more readily reduced than W(VI)/W(V) [53]. Electrostatic potential (ESP) calculations for VW_5 , V_2W_4 , and V_3W_3 indicate that the electron cloud density at the V–O–W bridging oxygen sites is significantly enhanced (Figs. 2(a)–2(c)). Consequently, V_3W_3 possesses the largest number of basic and reducible sites, exhibiting the strongest PCET activity. Accordingly, when Lindqvist-type POMs are spin-coated onto the surface of SAMs as a post-treatment agent, the V(V) centers accept electrons donated by nitrogen atoms in the SAMs and undergo reduction, while the V–O–W bridging oxygen sites with high electron density act as basic centers that abstract protons from the PA groups. Concerted electron and proton transfer drives the PCET process (Fig. 2(d)).

After hydrogen abstraction by the POMs, the exposed oxygen atoms in the PA groups form hydrogen bonds with hydroxyl groups on the surface of ITO, promoting transition of the anchoring mode from bidentate to tridentate and significantly enhancing the interfacial anchoring stability. The formation of hydrogen bonds is evidenced by the characteristic Raman peak of the –OH group ($\approx 3270\text{ cm}^{-1}$) [54]. Upon hydrogen bond formation, the polarizability of the O–H bond decreases, resulting in diminished Raman intensity. Raman mapping reveals that compared with the pristine SAM film, after treatment with VW_5 ,

V_2W_4 , and V_3W_3 , the –OH signals are markedly attenuated (Fig. 2(e)–2(h))), where the most pronounced intensity decrease is observed for V_3W_3 , indicating the strongest hydrogen-bonding interaction with ITO.

2.3 V_3W_3 enhancement of SAM anchoring effect

To further verify proton transfer between V_3W_3 and the SAM, the system was evaluated using nuclear magnetic resonance (NMR). The pristine SAM was used as the control and SAM/ V_3W_3 as the target. The ^{31}P -NMR spectrum (Fig. S10(a) in the ESM) reveals the emergence of a doublet signal, accompanied by a pronounced upfield shift upon V_3W_3 treatment, indicating a significant change in the chemical environment of phosphorus. This is attributed to proton abstraction from the PA groups by V_3W_3 . The corresponding upfield shift of the P–O–H peaks in the ^1H -NMR spectrum (Fig. S10(b) in the ESM) further corroborates proton transfer between V_3W_3 and the SAM. XPS was used to analyze the shape and components of the O 1s peaks before and after V_3W_3 modification (Figs. 3(a) and 3(b)). The variations in the O 1s peaks before and after V_3W_3 modification are presented in Table S1 in the ESM [55]. Quantitative comparison of the peak area ratios for the bidentate versus tridentate coordination states revealed that the proportion of tridentate anchoring increased significantly from 29.93% to 53.98% after V_3W_3 modification (Fig. 3(c)). This compositional evolution unambiguously demonstrates that V_3W_3 -mediated proton transfer drives conversion of the PA anchoring groups from a bidentate to a tridentate configuration.

The P signal represents the SAM, whereas the Sn signal corresponds to the underlying ITO substrate. Previous studies have indicated that desorption of the SAM exposes the underlying ITO substrate, increasing the intensity of the Sn signal, whereas a robustly anchored SAM effectively masks the substrate signal [54]. Thus, variations in the P/Sn ratio following rinsing with DMF serve

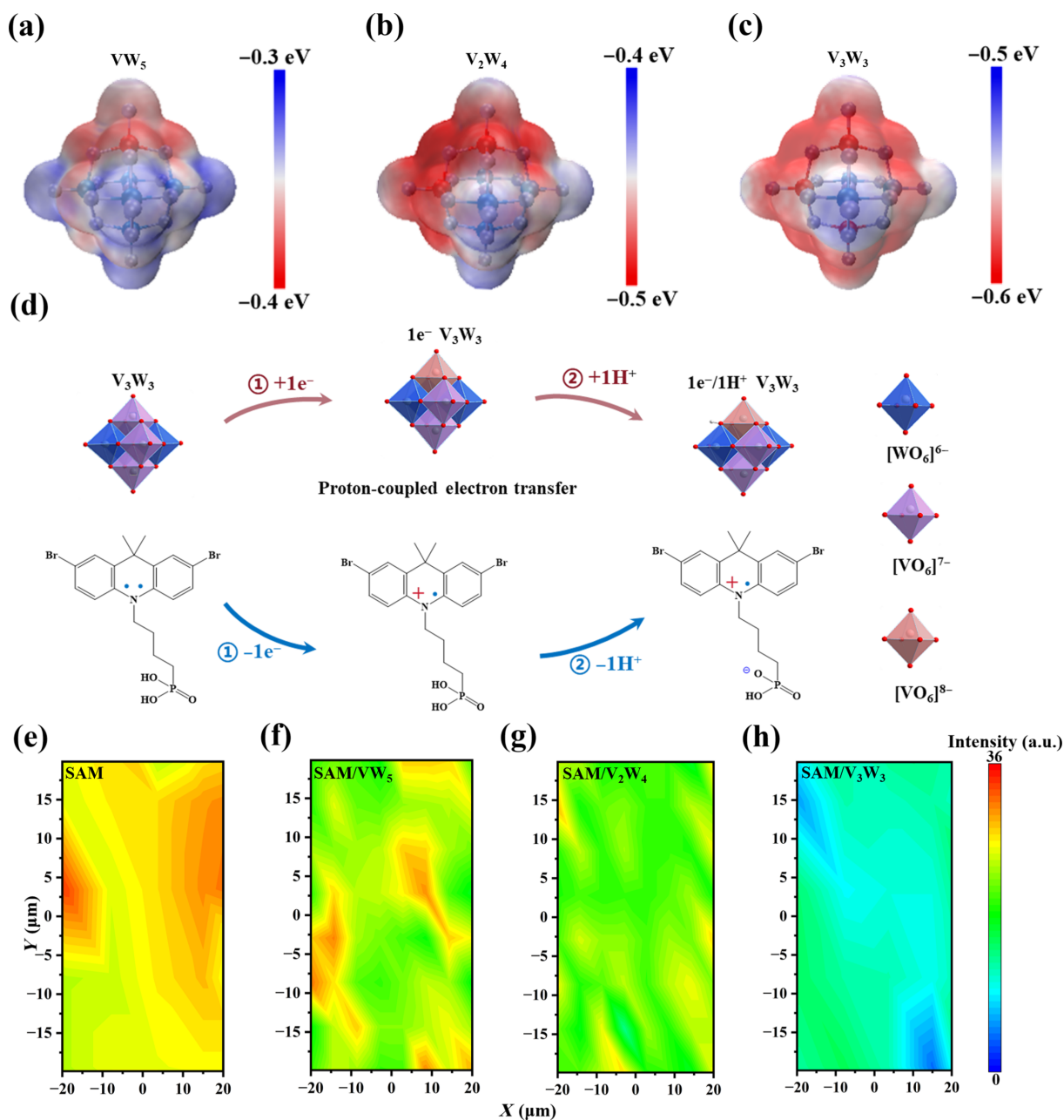


Figure 2 ESP distribution of (a) VW_5 , (b) V_2W_4 , and (c) V_3W_3 . (d) Schematic illustration of the PCET reaction pathway. Raman mappings of the characteristic $-OH$ groups on (e) pristine SAM, (f) SAM/ VW_5 , (g) SAM/ V_2W_4 , and (h) SAM/ V_3W_3 .

as a metric of the anchoring efficacy of the SAM (Fig. 3(d)). Notably, the pristine SAM underwent severe desorption after rinsing with DMF, where the P/Sn ratio decreased from 3.9% to 2.7%, corresponding to a SAM desorption rate of approximately 30.7%. In contrast, the P/Sn ratio of SAM/ V_3W_3 changed minimally during rinsing with DMF (from 3.6% to 3.4%), where only 5.6% SAM desorption was observed. These results demonstrate that V_3W_3 -mediated proton transfer drives the transition of the SAM anchoring configuration from bidentate to tridentate, reducing the DMF-induced SAM desorption rate from 30.7% to 5.6%. This significantly enhances the stability of the SAM-ITO interface and its resistance to solvent erosion, thereby establishing a durable interfacial base for the ensuing solution-based deposition of PVK films.

The proposed reaction mechanism is schematically depicted in

Fig. 3(e). In the pristine SAM layer, a substantial fraction of PAs retain bidentate binding rather than adopting deprotonated tridentate binding. These bidentate-binding PAs exhibit weaker affinity toward the substrate, rendering the SAM layer susceptible to dissolution or displacement during subsequent spin-coating of the PVK precursors in highly polar solvents, such as DMF. Localized desorption of the SAM at the buried interface ultimately induces defect formation, compromising the structural integrity of the deposited film. Upon treatment with V_3W_3 , the PA groups undergo proton transfer, and the exposed oxygen atoms form hydrogen bonds with the $-OH$ groups on the ITO surface. This drives the transition from unstable bidentate to stable tridentate binding, thereby preventing SAM detachment during subsequent PVK deposition. This suppresses the formation of interfacial voids and defects, and provides a uniform and stable template for PVK

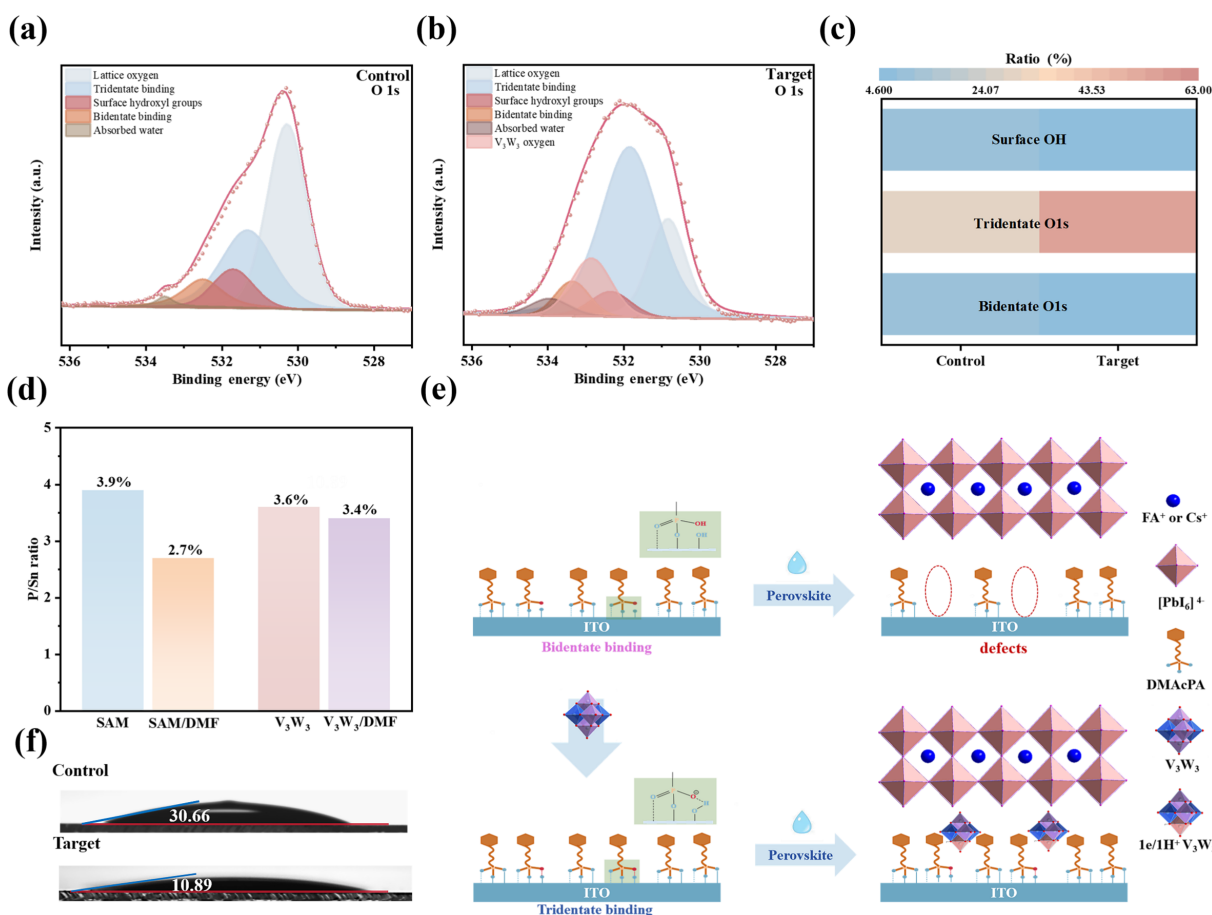


Figure 3 XPS O 1s spectra of (a) SAM and (b) SAM/V₃W₃ modified ITO surfaces. (c) The area ratios of the characteristic O 1s peaks. (d) Changes in the P/Sn ratio of SAM and SAM/V₃W₃ upon DMF rinsing. (e) Schematic of the V₃W₃ enhanced SAM anchoring mechanism. (f) Contact angles of PVK precursor on SAM and SAM/V₃W₃ films.

crystallization. Furthermore, upon incorporating V₃W₃, the contact angle of the PVK precursor decreased from 30.66° to 10.89° (Fig. 3(f)), indicating that V₃W₃ enhances the hydrophilicity of the SAM and facilitates the formation of a denser film.

2.4 Effect of V₃W₃ on HTL/PVK interface

The influence of V₃W₃ incorporation on the crystallinity of the PVK layer was examined using XRD [56] (Fig. S13 in the ESM). The intensity of the characteristic reflection at 14.1°, assigned to the (100) crystallographic plane of PVK, increased noticeably following V₃W₃ modification, signifying enhanced crystalline order within the film. This structural improvement was independently validated by high-resolution transmission electron microscopy imaging (Fig. S14 in the ESM). The surface morphology of the PVK films was subsequently inspected using scanning electron microscopy (SEM). To accentuate the grain-boundary contrast, post-acquisition image enhancement was applied to the micrograph in Fig. 4(a). The void density of the target film was substantially reduced relative to that of the control. Concomitantly, the average grain dimension of the target expanded from approximately 540 to 850 nm (Fig. S15 in the ESM). Cross-sectional SEM imaging (Fig. S16 in the ESM) further revealed that the target established more intimate and continuous contact with the underlying HTL, whereas the control suffered pronounced interfacial voids and irregular contact. These morphological advances are rationalized by the ability of V₃W₃ to promote the assembly of a dense, defect-less SAM layer on the ITO

surface, which not only suppresses interfacial void nucleation but also furnishes a uniform platform that guides high-quality PVK crystallization.

Beyond these features, the oxygen-rich architecture of V₃W₃ also induces some degree of defect passivation. FTIR spectroscopy verified chemical interaction between V₃W₃ and Pb²⁺ (Fig. S17 in the ESM). Vibrational modes were observed at 981.77 and 930.03 cm⁻¹ in the FTIR spectrum of the pristine V₃W₃ host. Upon co-processing with PbI₂, these bands downshifted to 978.17 and 926.24 cm⁻¹, respectively, indicating the formation of a coordinative bond between V₃W₃ and PbI₂. XPS corroborated this passivation scenario, in which the peaks in the Pb 4f core-level spectrum of the V₃W₃-treated film appeared at lower binding energies compared with those of the control (Fig. S18 in the ESM). The concentration of trap states within PVK was quantified by space-charge-limited current analysis using a hole-only device (ITO/DMAcPA/PVK/PTAA/Cu) (Fig. S19 in the ESM). V₃W₃ treatment lowered the trap-filling limit voltage (V_{TFL}) from 0.73 to 0.35 V. Based on the equation $N_t = 2\epsilon_0\epsilon_r V_{TFL}/qL^2$, the calculated defect density decreased from 2.08×10^{16} to 1.01×10^{16} cm⁻³.

The optoelectronic quality at the buried PVK interface was probed through steady-state photoluminescence (PL) and time-resolved photoluminescence (TRPL) measurements [57]. Pronounced PL quenching was observed for the PVK layer grown on the SAM/V₃W₃ (Fig. 4(b)), indicating accelerated interfacial charge extraction. TRPL analysis yielded an average carrier lifetime

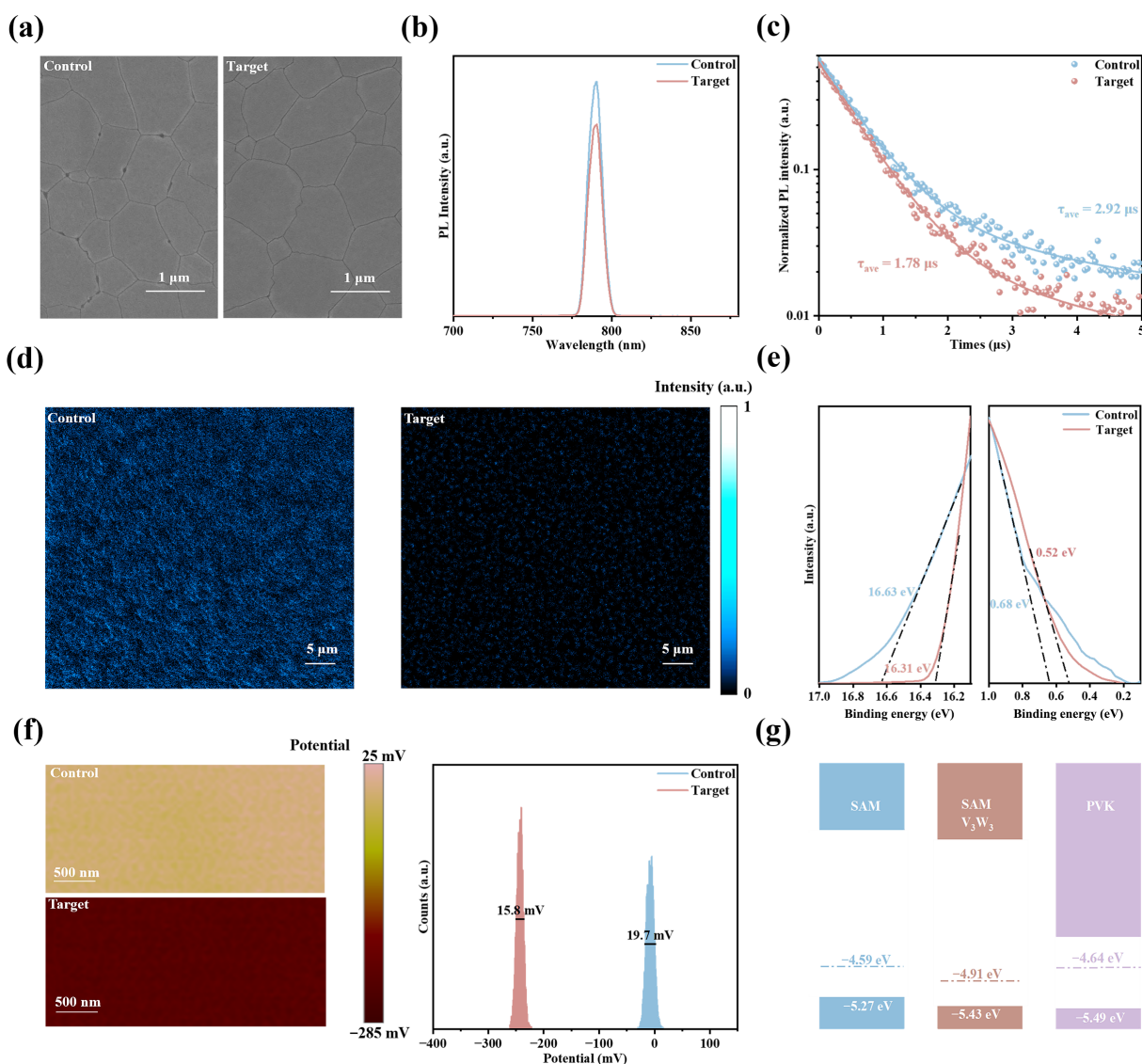


Figure 4 (a) SEM images, (b) PL spectra, (c) TRPL spectra, and (d) PL mapping images of PVK buried interfaces based on SAM and SAM/V₃W₃. (e) UPS spectra, (f) KPFM images and surface potential distributions, and (g) schematic energy level alignment of SAM and SAM/V₃W₃.

(τ_{ave}) of 1.78 μs for the target, a sharp decrease from the 2.92 μs recorded for the control (Table S2 in the ESM and Fig. 4(c)). This shortening of the excited-state lifetime implies successful reduction of the number of non-radiative recombination centers at the buried interface following V₃W₃ treatment. PL mapping (Fig. 4(d)) reveals uniformly weaker emission across the V₃W₃-treated films, mirroring the ensemble spectroscopic trend. The origin of these improvements lies in reorganization of the V₃W₃-treated SAMs into a more ordered and robust monolayer, which improves the crystallization quality of PVK and reduces the density of interfacial trap states.

UPS was utilized to track how V₃W₃ modification alters the work function and energy levels of the SAM and PVK. The Fermi levels (E_F), calculated as $E_F = E_{\text{cutoff}} - 21.22 \text{ eV}$, are shown in Fig. 4(e) [58]. The conduction band (CB) edge of the SAM shifted downward by 0.16 eV after V₃W₃ treatment, narrowing the energy gap between the E_F and the CB from 0.68 to 0.52 eV. KPFM measurements (Fig. 4(f)) recorded an average contact potential difference (CPD) of −9 mV for the pristine SAM, which dropped to −240 mV upon V₃W₃ treatment. The decrease in the CPD corresponds to an

increase in the work function, indicating a downward shift of the E_F level upon V₃W₃ treatment, facilitating more efficient hole extraction and transport. This correlation was further corroborated by UPS measurements (Fig. 4(g)). The attainment of a larger work function promotes more favorable energy-level alignment at the HTL/PVK junction, fostering efficient hole transfer, which is essential for achieving high fill factors (FF) and open-circuit voltages (V_{OC}) in PSCs.

2.5 Optimization of photovoltaic performance and stability of PVK

To evaluate how V₃W₃ influences the photovoltaic performance, PSCs were constructed with the layer sequence ITO/DMAcPA/PVK/PCBM/BCP/Cu (Fig. S20 in the ESM). Systematic screening of V₃W₃ concentration revealed 0.5 mg·mL^{−1} to be the ideal loading (Fig. S21 in the ESM). Representative J - V characteristics obtained under both forward and reverse voltage sweeps are presented in Figs. 5(a) and 5(b). The control PSC delivered a PCE of 23.68%, with a short-circuit current density (J_{SC}) of 25.10 mA cm^{−2}, an FF of

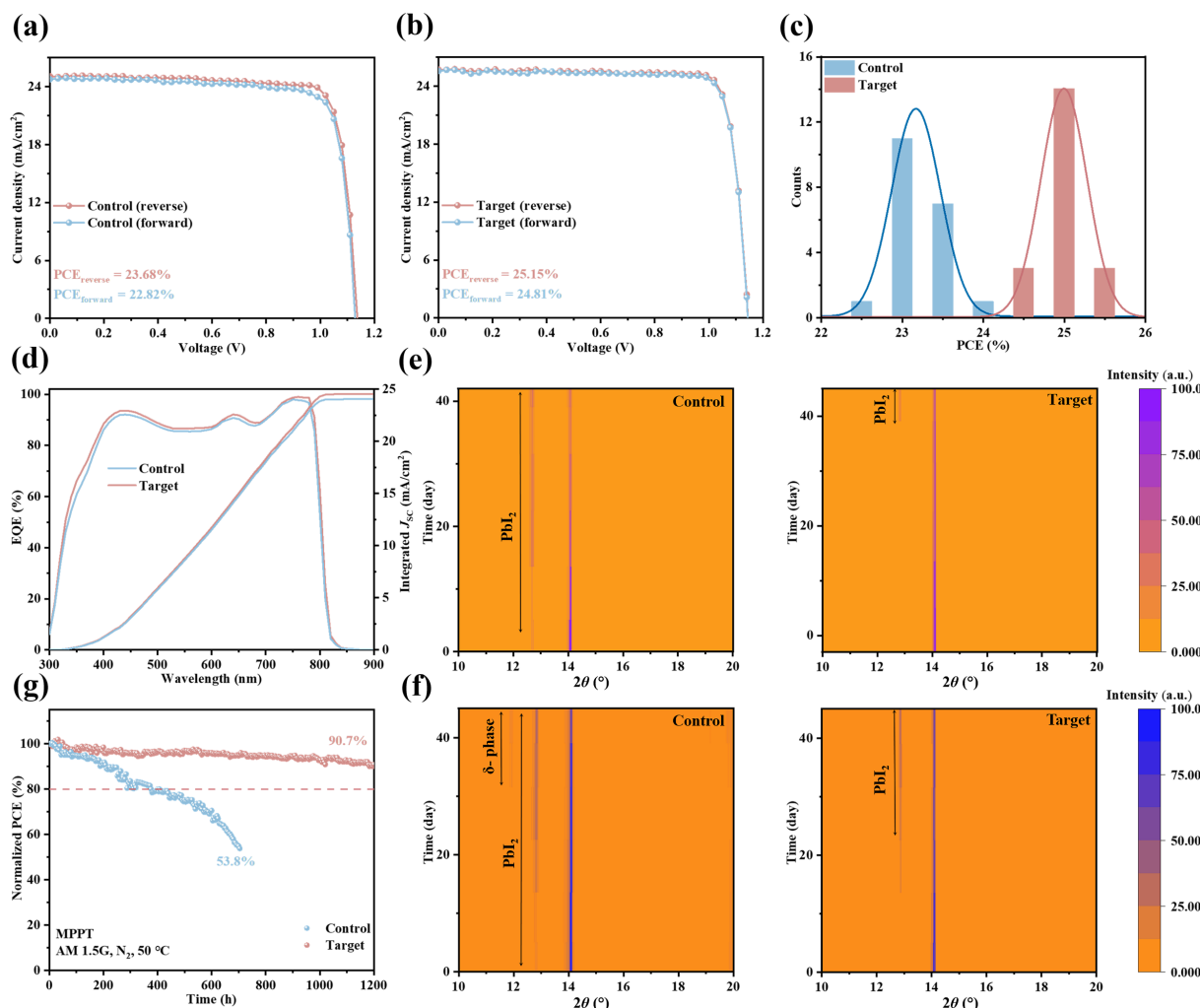


Figure 5 $J-V$ curves of the (a) control and (b) target PSCs under forward and reverse scans. (c) PCE frequency distribution histograms under reverse (1.2 V→0 V) direction and (d) EQE spectra with integrated photocurrent of the control and target PSCs. Corresponding XRD evolution patterns under continuous (e) thermal aging (N₂, 85 °C) and (f) humid atmosphere (30%–40% relative humidity, room temperature), respectively. (g) MPPT of unencapsulated control and target PSCs under continuous AM1.5G in N₂ atmosphere.

82.97%, and a V_{OC} of 1.137 V. In contrast, the V_3W_3 -modified PSC attained a markedly improved PCE of 25.15%, alongside a J_{SC} of 25.73 mA·cm⁻², an FF of 85.44%, and a V_{OC} of 1.144 V. Furthermore, the hysteresis index dropped from 3.63% for the control to merely 1.35% for the target device. This performance enhancement proved universal across a batch of 20 independently fabricated PSCs (Fig. 5(c) and Fig. S22 in the ESM). The external quantum efficiency (EQE) was determined to cross-validate the J_{SC} [59]. Integration of the EQE data yielded J_{SC} values of 24.04 and 24.53 mA·cm⁻² for the control and target devices, respectively, in close concordance with the $J-V$ data (Fig. 5(d)). The PCE improvement originates from the concerted enhancement of the J_{SC} , FF, and V_{OC} , which is intrinsically rooted in the PCT effect of V_3W_3 . This effect stabilizes the SAM layer, thus enabling comprehensive optimization of the buried interface. The steady-state operational behavior was probed via MPPT (Fig. S23 in the ESM). The control PSC settled at a stabilized photocurrent of 23.84 mA·cm⁻² and a steady-state power output of 23.12%, whereas the V_3W_3 -treated PSC registered 24.51 mA·cm⁻² and 24.75%, demonstrating superior steady-state operation.

The dark $J-V$ measurement of the target device (Fig. S24 in the ESM) is significantly suppressed compared to that of the control

device, which directly confirms the effective suppression of non-radiative recombination by V_3W_3 . The dependence of both V_{OC} and J_{SC} on the illumination intensity was examined (Figs. S25 and S26 in the ESM). For the control device, the V_{OC} versus logarithmic light intensity plot yielded a slope of $1.62k_B T/q$ (k_B = Boltzmann constant, T = absolute temperature, q = elementary charge). This slope narrowed to $1.26 k_B T/q$ upon V_3W_3 incorporation. Concomitantly, the short-circuit ideality factor increased from 0.959 to 0.979, edging closer to 1. Such trends signal pronounced mitigation of the Shockley–Read–Hall recombination in the target PSCs. The above improvements in the electrochemical properties originate from optimization of the carrier transport by V_3W_3 , where the underlying mechanism was systematically elucidated through Mott-Schottky analysis and electrochemical impedance spectroscopy (EIS). Specifically, Mott-Schottky profiling (Fig. S27 in the ESM) revealed an enlargement of the built-in potential (V_{bi}) from 0.80 to 0.85 V, which amplifies the internal driving force for exciton dissociation and charge extraction. The Nyquist plots from EIS (Fig. S28 in the ESM) further prove an increase in the recombination resistance (R_{rec}) from 1095 to 1707 Ω , providing direct evidence of curtailed interfacial non-radiative losses and a concomitant V_{OC} boost. Collectively, V_3W_3 engineering orchestrates

a multifaceted improvement in interfacial charge dynamics: it strengthens the V_{bi} and suppresses carrier recombination, culminating in a substantial leap in the overall figure-of-merit of the device.

Beyond PCE, long-term durability is a prerequisite for commercial translation. The stability of the PVK film was, therefore, benchmarked under accelerated aging protocols: continuous thermal stress at 85 °C under N_2 (Fig. S29 in the ESM) and exposure to ambient atmosphere at 30%–40% relative humidity (Fig. S30 in the ESM). After 90 days, the control film underwent severe morphological degradation, whereas the V_3W_3 -treated film retained its initial texture under both thermal and moist environments, attesting to its robust anti-aging characteristics. The phase integrity was monitored by XRD analysis over 42 days (Figs. 5(e) and 5(f)). Under thermal loading, the α -FAPbI₃ (001) reflection of the control film changed progressively, accompanied by the gradual appearance of a PbI₂ signature at $2\theta = 12.7^\circ$, a hallmark of thermally induced PVK decomposition. Conversely, the intensity of the (001) peak remained constant throughout the test for the V_3W_3 -treated film, where PbI₂ was detectable only after day 40, evidencing markedly retarded phase degradation. Under humidity stress, the intensity of the (001) peak of α -FAPbI₃ again declined steeply for the control film, together with the emergence of two peaks near 11.8° and 12.7°, ascribed to the inactive δ -phase and PbI₂, respectively. In comparison, for the target film, the (001) reflection merely exhibited mild weakening, without any discernible formation of inactive phases, confirming superior humidity tolerance.

Finally, the stability of unencapsulated PSCs was tracked under various stressors (Figs. S31–S33 in the ESM). Following 90 days of aging under humid air, the V_3W_3 -treated PSC preserved 84.1% of its initial PCE, whereas that of the control PSC plummeted to < 71.9%. Under thermal aging at 85 °C under N_2 for 1000 h, the target PSC retained 89.6% of its starting PCE, versus 72.0% for the control PSC. At 25 °C under N_2 , the target PSC retained > 95% of its initial PCE after 1000 h, outperforming the control PSC (< 85%). The operational stability was further assessed via MPPT under continuous AM1.5G illumination under N_2 (Fig. 5(g)). The PCE of the control PSC declined by 50% within roughly 600 h, whereas the target PSC sustained 90.7% of its initial PCE after 1200 h of uninterrupted operation. This extraordinary endurance is ascribed to the reinforced SAM–ITO adhesion imparted by V_3W_3 , which suppresses interfacial decomposition and ensures durable hole extraction throughout extended device operation.

3 Conclusions

V_3W_3 was utilized as post-treatment agent for SAMs. Leveraging a PCET pathway, proton transfer from V_3W_3 to the SAM concurrently fosters hydrogen-bonding interactions at the SAM–ITO interface and triggers a configurational shift in the surface anchoring mode from bidentate to tridentate. Consequently, the fractional population of tridentate-bound species increased markedly from 29.93% to 53.98%. This structural reorganization substantially fortifies the SAM against solvolytic removal under polar conditions, as evidenced by the drastic suppression of the DMF-mediated desorption rate from 30.7% to merely 5.6%. Beyond these achievements, V_3W_3 mediates effective defect passivation at the buried interface, refines the energetic alignment between adjacent layers, accelerates hole collection, and

quenches non-radiative recombination losses. The PSC engineered with this V_3W_3 modification delivered a PCE of 25.15% and a V_{OC} of 1.144 V, representing a considerable advance relative to the 23.68% recorded for the control. Equally notable is the markedly enhanced operational stability. The unencapsulated PSC preserved 95.8% of its initial PCE after 1000 h of storage under inert atmosphere and sustained 90.7% of its original PCE after 1200 h of uninterrupted MPPT. These findings underscore the importance of judicious control over SAM anchoring as a design strategy for realizing PSCs with simultaneously high PCE and exceptional durability.

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Data availability

All data needed to support the conclusions in the paper are presented in the manuscript and the Electronic Supplementary Material. Additional data related to this paper may be requested from the corresponding author upon request.

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Declaration of competing interest

All the contributing authors report no conflict of interests in this work.

Author contribution statement

J. Y. W.: Methodology, investigation, formal analysis and writing original draft. Y. P.: Software, formal analysis. W. L. C.: Funding acquisition, supervision, writing – reviewing & editing. F. Y. J.: Data curation, investigation. Q. W. T.: Writing – review & editing, supervision, project administration, funding acquisition. All the authors have discussed the results and approved the final manuscript.

Use of AI statement

None.

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