Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# *Supporting Information*

## Multifunctional Anthraquinone-Sulfonic Potassium Salts Passivates the Buried Interface for Efficient and Stable Planar Perovskite Solar Cells

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This file includes **Figure S1-S12** and **Table S1-S3**:

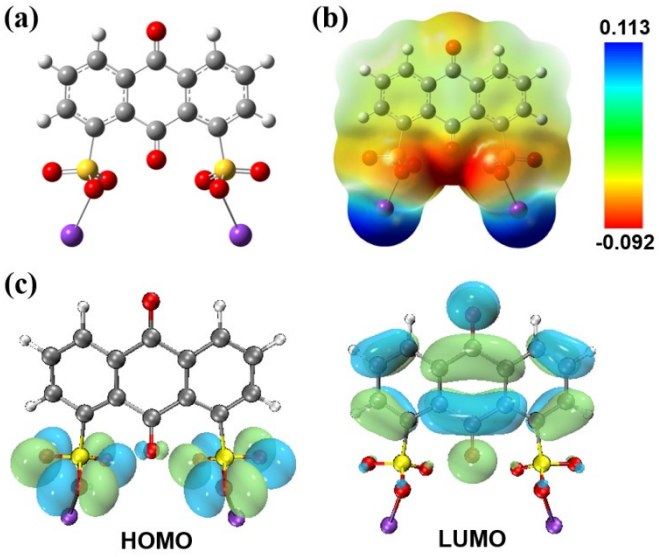



**Figure S1.** (a) Molecular structure, (b) electrostatic surface potential map, and (c) calculated frontier molecular orbitals of ASPS molecule.

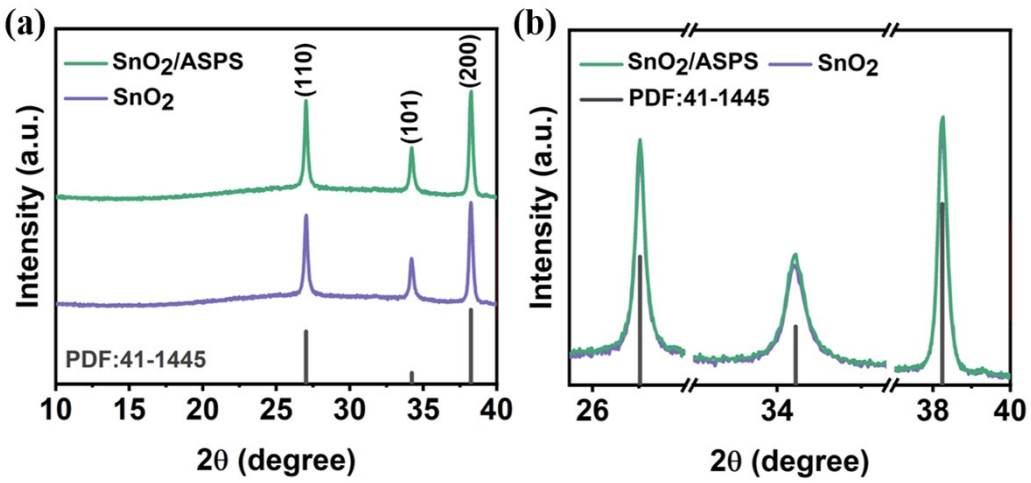



**Figure S2.** XRD patterns of $SnO_2$ film without and with ASPS modification.

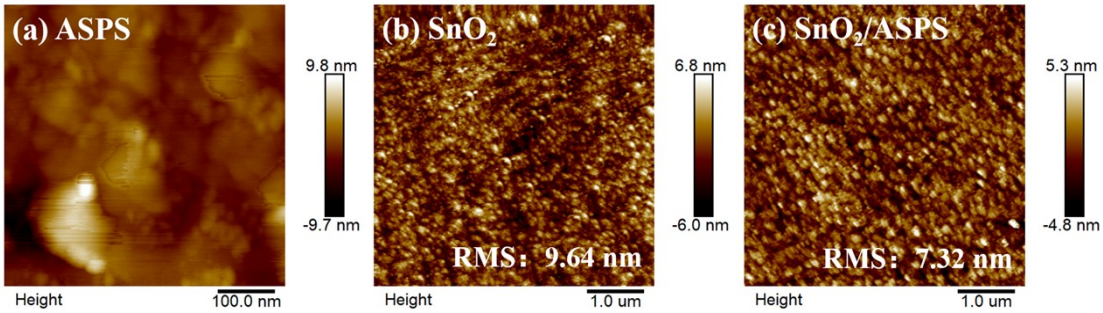



**Figure S3.** AFM images of (a) ASPS, (b) $SnO_2$ and (c) ASPS-modified $SnO_2$ on glass substrates, respectively.

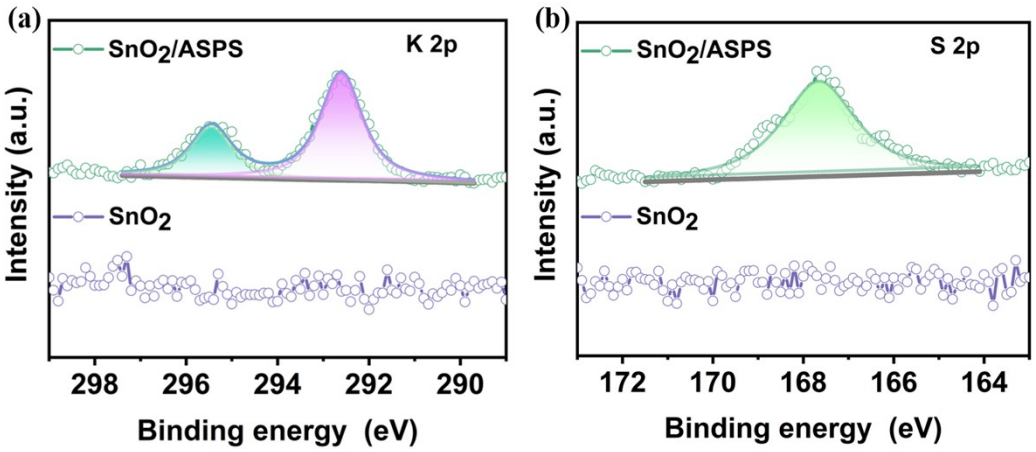



**Figure S4.** (a) K 2p, and (c) S 2p XPS spectra of $SnO_2$ and $SnO_2$/ASPS substrates, respectively.

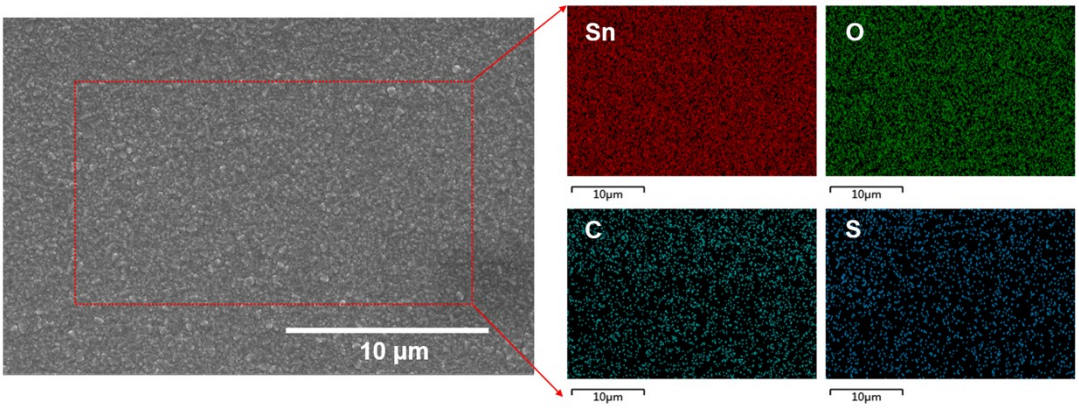



**Figure S5.** Top-view SEM and corresponding energy dispersive spectroscopy (EDS) mapping of $SnO_2$/ASPS substrate, respectively.

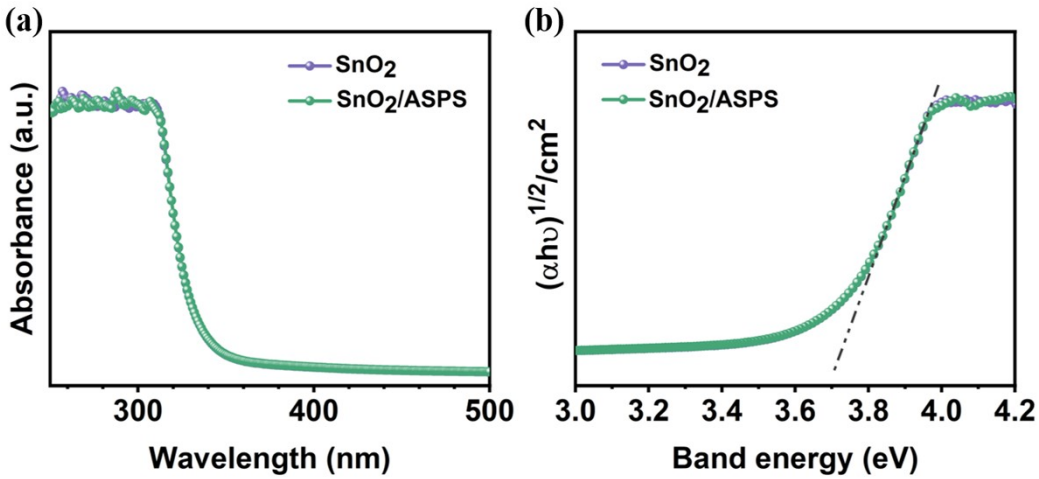



**Figure S6.** (a) Optical absorbance and (d) corresponding Tauc plots of $SnO_2$ film without or with ASPS modification.

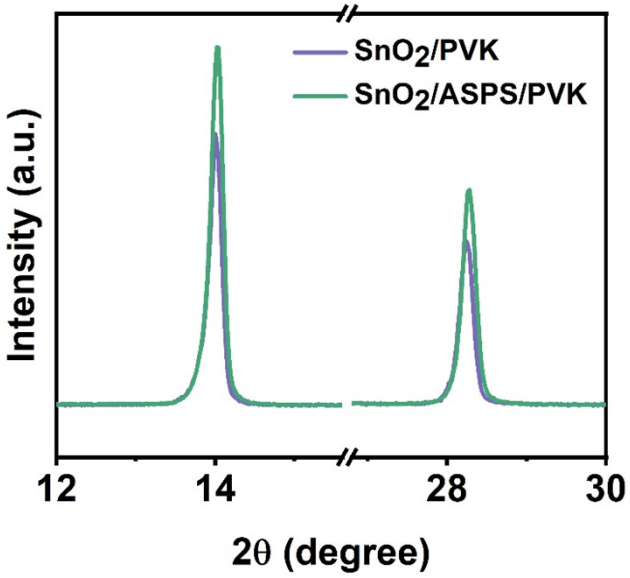



**Figure S7.** Region amplified XRD pattern of PVK films deposited on $SnO_2$ and $SnO_2$/ASPS substrates.

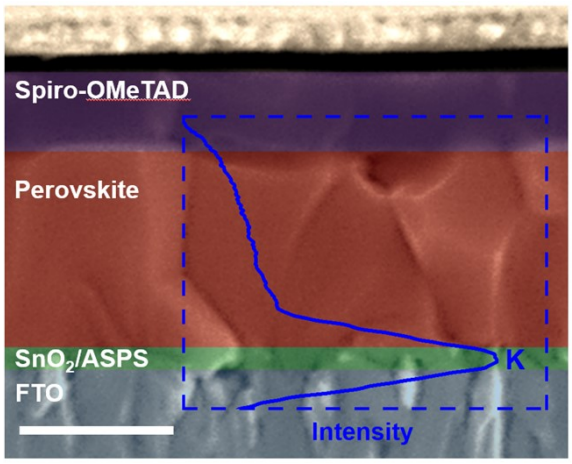



**Figure S8.** Elemental scanning in a liner mode through the cross-section of $SnO_2$/ASPS/PVK. Scale bar: 500 nm.

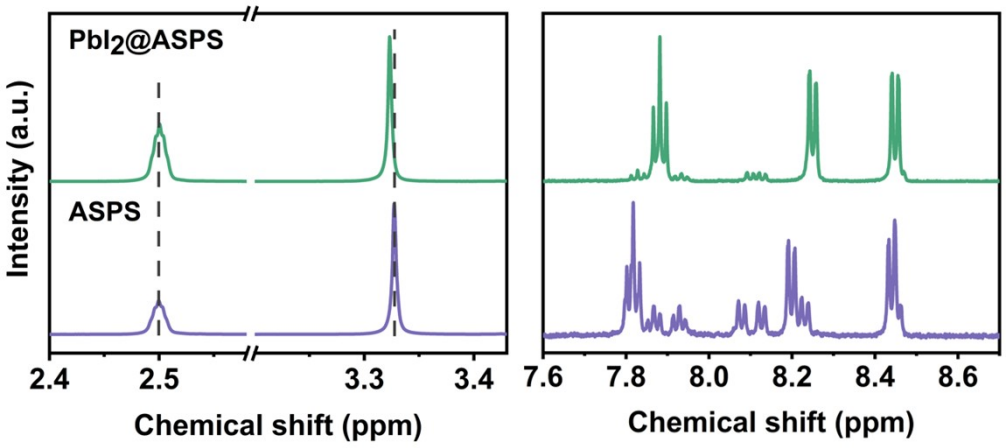



**Figure S9.** Liquid-state $^{1}$H NMR spectra of pure ASPS and $PbI_2$@ASPS dissolving in DMSO-$d_6$, respectively.

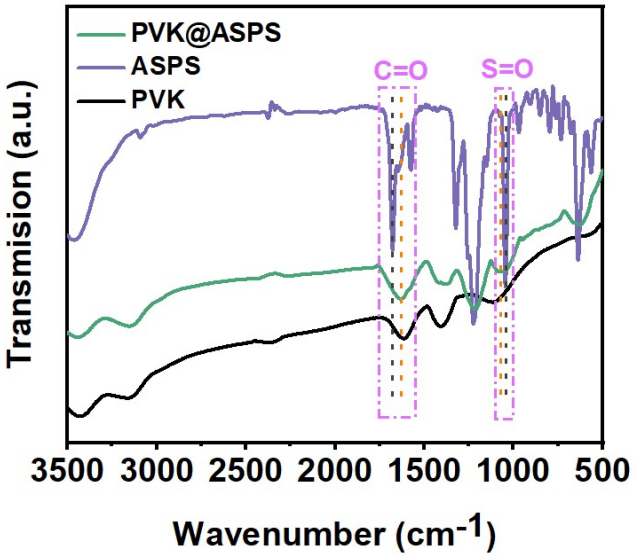



**Figure S10.** FTIR spectra of PVK, pure ASPS powder, and PVK@ASPS, respectively.

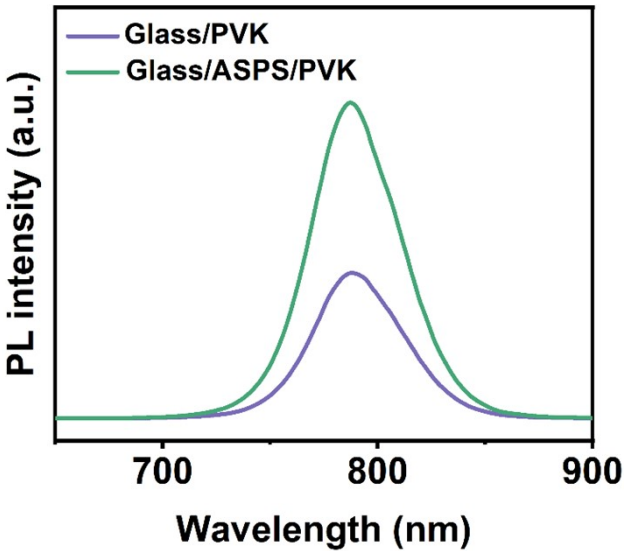



**Figure S11.** The steady-state PL spectra of PVK films deposited on $SnO_2$ and $SnO_2$/ASPS substrates.

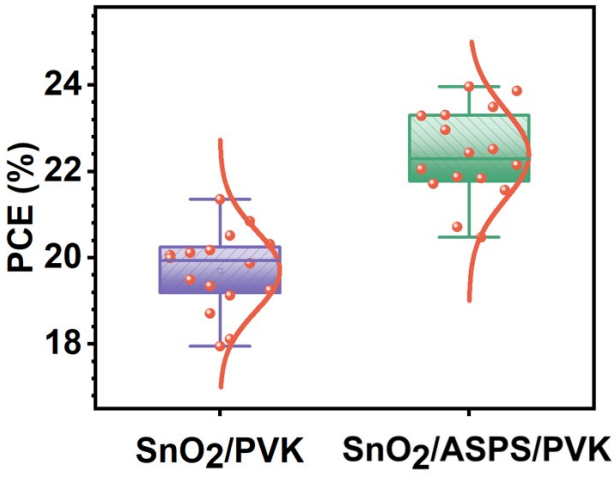



**Figure S12.** Statistical distribution of PCE of the controlled and optimized PSCs. The statistical data were collected from 16 cells for each case.

**Table S1.** The photovoltaic parameters of the champion devices with different concentrations of ASPS.

| ASPS (mg/mL) | *V*oc (V) | *J*sc (mA/cm$^2$) | FF (%) | PCE (%) |
|---|---|---|---|---|
| 0.0 | 1.10 | 24.47 | 79.37 | 21.36 |
| 0.25 | 1.13 | 24.51 | 80.83 | 22.39 |
| 0.5 | 1.16 | 24.57 | 81.98 | 23.36 |
| 0.75 | 1.17 | 24.76 | 82.70 | 23.96 |
| 1.0 | 1.15 | 24.43 | 79.83 | 22.43 |

**Table S2.** The photovoltaic parameters of the champion devices with AD, ADA, and ASPS, respectively.

| Sample | | *V*oc (V) | *J*sc (mA/cm$^2$) | FF (%) | PCE (%) |
|---|---|---|---|---|---|
| AD | FS | 1.12 | 24.59 | 78.83 | 21.71 |
| | RS | 1.16 | 24.61 | 81.32 | 23.21 |
| ADA | FS | 1.13 | 24.67 | 80.03 | 22.31 |
| | RS | 1.16 | 24.70 | 82.86 | 23.74 |
| ASPS | FS | 1.16 | 24.75 | 80.16 | 23.01 |
| | RS | 1.17 | 24.76 | 82.70 | 23.96 |

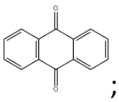
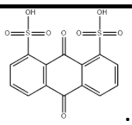
Anthracenedione (AD):  ; 1,8-Anthracenedisulfonic acid (ADA):  .

**Table S3.** Initial photovoltaic parameters of the stability test device under reverse scanning.

| | | *V*oc (V) | *J*sc (mA/cm$^2$) | FF (%) | PCE (%) |
|---|---|---|---|---|---|
| Storage stability | 0.0 | 1.09 | 24.45 | 78.56 | 20.94 |
| | 0.75 | 1.16 | 24.74 | 80.96 | 23.23 |
| Thermal stability | 0.0 | 1.08 | 24.46 | 78.43 | 20.72 |
| | 0.75 | 1.15 | 24.70 | 81.12 | 23.04 |

| | | | | | |
|---|---|---|---|---|---|
| Light stability | 0.0 | 1.08 | 24.45 | 78.34 | 20.69 |
| | 0.75 | 1.14 | 24.73 | 80.70 | 22.75 |