Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2022

Multifunctional strategy of two-dimensional WS₂ modified absorbers for efficient planar perovskite solar cells

Qinghua Sun,^a Wanting Hu,^a Miao Yu,^a Fengyou Wang,^{ab} Xiaoyan Liu,^{ab} Lihua Yang,^{ab} Huilian Liu,^{*ab} Lin Fan^{**ab} and Lili Yang^{***ab}

- ^a Key Laboratory of Functional Materials Physics and Chemistry (Ministry of Education), College of Physics, Jilin Normal University, Changchun 130103, China
- ^b National Demonstration Center for Experimental Physics Education, Jilin Normal University, Siping 136000, China

* Correspondence: <u>lhl541@126.com</u> (H. Liu), <u>fanlin@jlnu.edu.cn</u> (L. Fan), <u>llyang1980@126.com</u> (L. Yang)



Figure S1. Cross-sectional SEM images of different absorbers: (a) PVK-C and (b) PVK-W.



Figure S2. FWHM and diffraction intensity of PVK-C and PVK-W films.



Figure S3. (a) UV-vis absorption spectra and (b) Tauc plots of perovskite films with and without WS₂ NSs. The E_g of the samples with and without WS₂ were calculated to be 1.578 and 1.583 eV, respectively, using the formula $\alpha hv = A (hv - E_g)^n$, where α is the absorption coefficient, hv is photon energy, A is a constant, and n varies according to allowed or forbidden direct and indirect transitions. The value n = 1/2 is employed in this case since the perovskite is regarded as a direct band-gap semiconductor.



Figure S4. (a) XPS spectra of PVK-C and PVK-W films. High-resolution XPS spectra of the corresponding samples: (b) Pb 4f and (c) I 3d.



Figure S5. (a) J-V curves of planar PSCs fabricated with the WS₂ concentrations of 0.00 mg/mL, 0.02 mg/mL, 0.04 mg/mL, and 0.08 mg/mL, respectively. (b) Photographs of dispersions fabricated using WS₂ of 0.00, 0.02, 0.04, 0.08, and 0.10 mg/mL.



Figure S6. (a)-(b) Stable current densities and PCEs measured under constant bias of 0.86 V (PVK-C device) and 0.92 V (PVK-W device).



Figure S7. EQE spectra of the best-performing planar devices based on PVK-C and PVK-W devices.

Dynamic parameters from TRPL curves.

| Samples | A_1 | $\tau_1(ns)$ | A_2 | $\tau_2(ns)$ |
|---------|-------|--------------|-------|--------------|
| PVK-C | 4104 | 8.3 | 2038 | 33.9 |
| PVK-W | 1005 | 2.8 | 490 | 22.8 |

Fitting parameters from EIS.

| Samples | Rs | R _{tr} | Rrec | $C_{ m tr}$ | Crec |
|---------|-------|------------------------|-------|-----------------------|----------------------|
| | (Ω) | (Ω) | (Ω) | (F) | (F) |
| РУК-С | 31.20 | 52.35 | 185.8 | 1.05×10^{-8} | 6.7×10 ⁻⁹ |
| PVK-W | 17.46 | 32.26 | 327.5 | 1.04×10 ⁻⁸ | 8.2×10 ⁻⁹ |

| PVK-W PSCs | $J_{\rm SC}$ | Voc | FF | Eff. |
|------------|-----------------------|-----------------|------------|------------------|
| | (mA/cm ²) | (V) | (%) | (%) |
| 1 | 22.82 | 1.10 | 78.86 | 19.89 |
| 2 | 23.52 | 1.12 | 77.03 | 20.43 |
| 3 | 23.25 | 1.10 | 75.25 | 19.36 |
| 4 | 23.15 | 1.11 | 78.63 | 20.24 |
| 5 | 23.35 | 1.11 | 78.12 | 20.32 |
| 6 | 23.65 | 1.12 | 78.92 | 21.03 |
| 7 | 23.11 | 1.10 | 77.09 | 19.64 |
| 8 | 23.94 | 1.14 | 75.52 | 20.74 |
| 9 | 24.12 | 1.13 | 76.58 | 20.96 |
| 10 | 24.23 | 1.13 | 76.31 | 20.87 |
| 11 | 23.71 | 1.09 | 75.96 | 19.80 |
| 12 | 23.59 | 1.10 | 76.66 | 20.03 |
| Average | 23.53 ± 0.41 | 1.11 ± 0.02 | 77.07±1.24 | 20.27 ± 0.53 |

Photovoltaic parameters of PVK-W PSCs. The J-V curves were measured in R-S under the AM 1.5G illumination. Average data were calculated from 12 devices for each condition.

| PVK-C PSCs | J _{SC} | Voc | FF | Eff. |
|------------|-----------------------|-----------|------------|------------|
| | (mA/cm ²) | (V) | (%) | (%) |
| 1 | 22.31 | 1.11 | 73.72 | 18.35 |
| 2 | 22.63 | 1.13 | 73.22 | 18.73 |
| 3 | 21.42 | 1.09 | 73.10 | 17.03 |
| 4 | 22.80 | 1.12 | 73.26 | 18.76 |
| 5 | 21.46 | 1.10 | 70.98 | 18.24 |
| 6 | 22.27 | 1.13 | 74.41 | 17.63 |
| 7 | 23.01 | 1.13 | 74.87 | 19.49 |
| 8 | 22.93 | 1.13 | 74.74 | 19.38 |
| 9 | 22.83 | 1.12 | 73.40 | 18.90 |
| 10 | 22.52 | 1.10 | 73.78 | 18.30 |
| 11 | 23.27 | 1.13 | 74.69 | 19.75 |
| 12 | 22.75 | 1.13 | 73.88 | 19.02 |
| Average | 22.51±0.56 | 1.11±0.02 | 73.67±1.01 | 18.63±0.75 |

Photovoltaic parameters of PVK-C PSCs. The J-V curves were measured in R-S under the AM 1.5G illumination. Average data were calculated from 12 devices for each condition.