Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.
This journal is © The Royal Society of Chemistry 2023

Supporting Information

Modification of back interfacial contact with MoO_3 layer in-situ introduced by Na_2S aqueous solution for efficient kesterite CZTSSe solar cells

Yue Jian, Tianliang Xie, Litao Han, Dongxing Kou, Wenhui Zhou, Zhengji Zhou, Shengjie Yuan, Yuena Meng, Yafang Qi, and Sixin Wu*.*

Key Laboratory for Special Functional Materials of MOE, National & Local Joint Engineering Research Center for High-efficiency Display and Lighting Technology, Collaborative Innovation Center of Nano Functional Materials and Applications, School of Materials, Henan University, Kaifeng 475004, P. R. China.

*E-mail: hlt@henu.edu.cn; wusixin@henu.edu.cn.

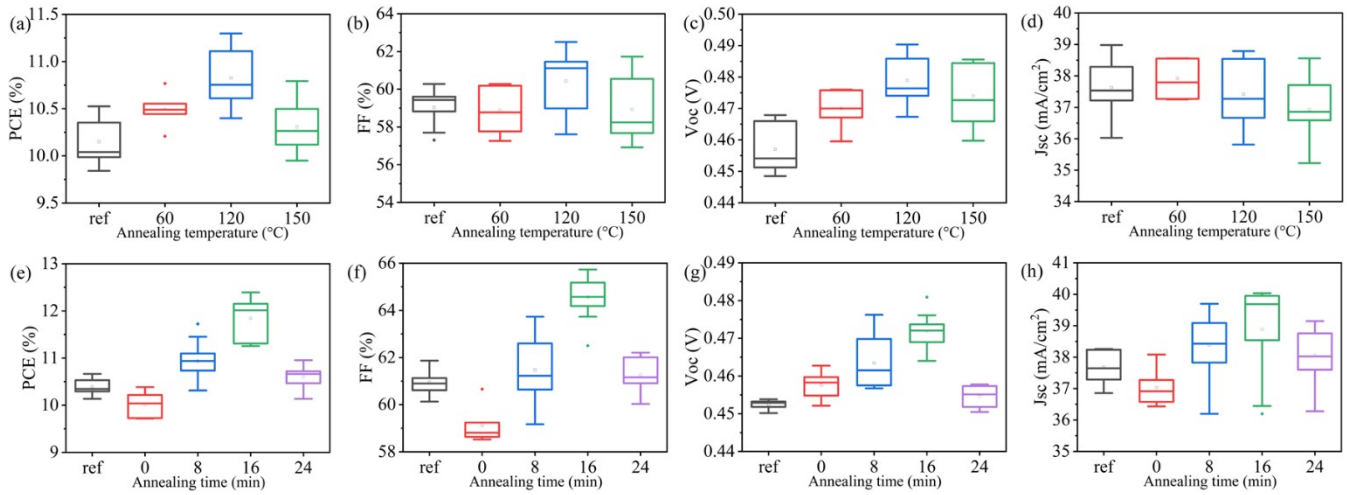

Figure S1. Photovoltaic parameters of the devices fabricated on the Mo substrate with Na_2S layer annealed at different temperature: a) PCE, b) FF, c) V_{OC} and d) J_{SC}, and annealed for different time: e) PCE, f) FF, g) V_{OC} and h) J_{SC}.

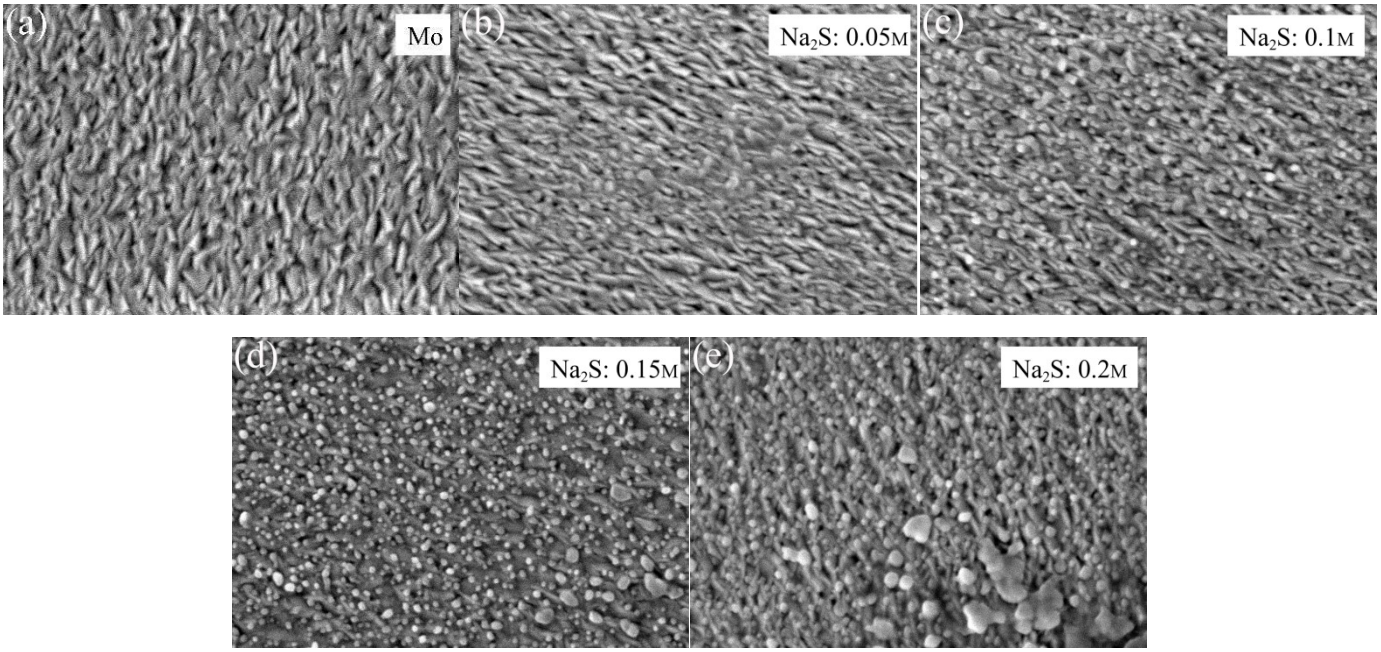

Figure S2. The morphologies of spin-coated Na_2S on Mo surface with various mole rations: a) 0 M, b) 0.05 M, c) 0.1 M, d) 0.15 M, e) 0.2 M.

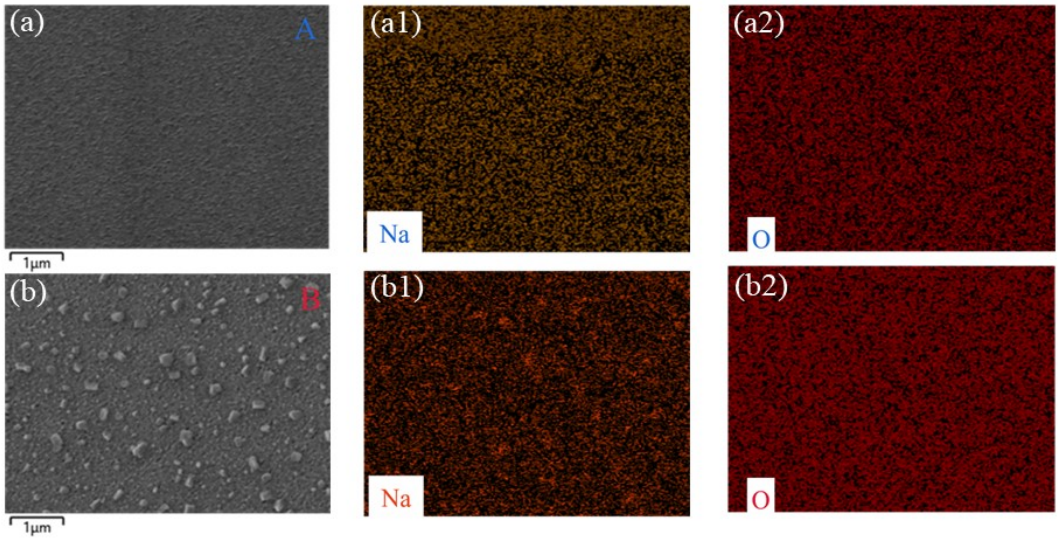

Figure S3. EDS maps of the substrate (a) A and (b) B.

Table S1. Quantitative EDX analysis of Na, Mo and O content for back contact surfaces of A and B.

Substrate	Mo	O	Na	S
A	88.94	11.06	0	0
B	76.37	21.26	1.39	0.98

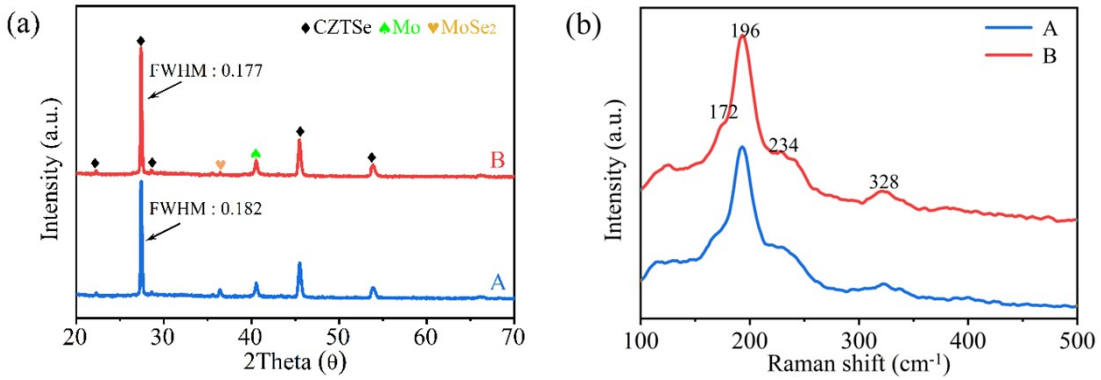

Figure S4. (a) XRD spectra of CZTSSe film without (A) and with (B) Na_2S layer. (b) Raman spectra of the film A and B. The intensity of (112) diffraction peaks of CZTSSe located at 27.18° (JCPDS#52-0868) increases a little on substrate B. And there is a narrowing of the FWHM from 0.182 for film A to 0.177 for film B, suggesting the improved crystalline quality. The crystalline quality is further revealed by Raman measurement. In addition, XRD and Raman spectroscopy demonstrates that the Na_2S aqueous solution does not cause the formation of secondary phase in the absorber layer.

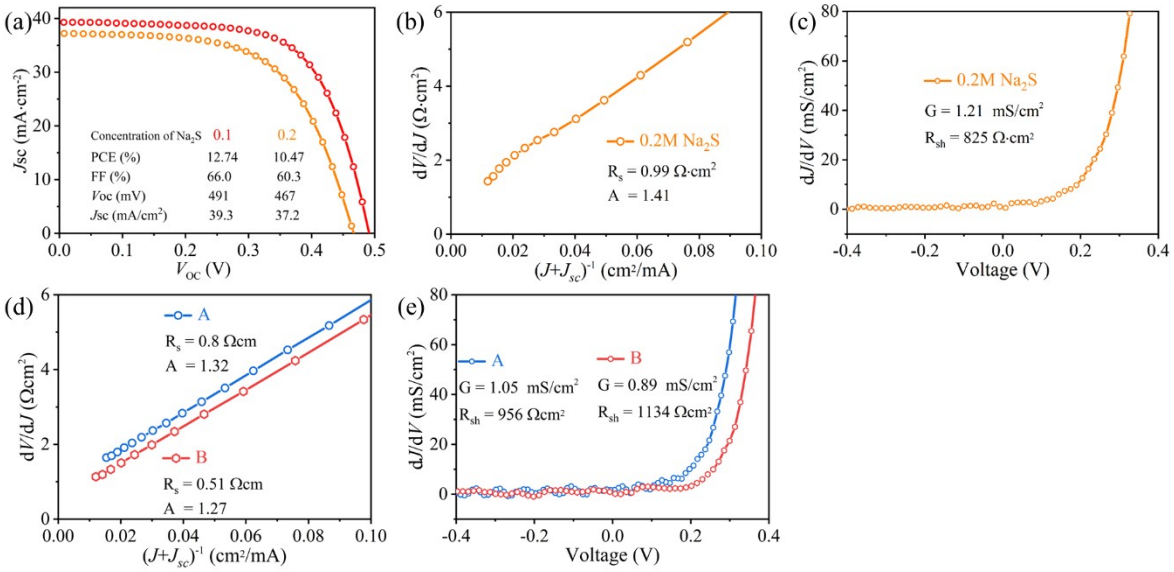

Figure S5 . (a) J-V curves of the champion devices prepared on the substrates treated with 0.1 M and 0.2 M Na_2S; (b) dV/dJ vs $(J + Jsc)^{-1}$ and (c) dJ/dV vs V redrawn from the standard light J–V curves of the champion device prepared on the substrates treated with 0.2 M Na_2S; Plots of (d) dV/dJ vs $(J + Jsc)^{-1}$ and (e) dJ/dV vs V redrawn from the standard light J–V curves of device A and B (0.1 M Na_2S).

Table S2. The photovoltaic parameters of the champion device prepared on the substrates treated with 0.1 M and 0.2 M Na_2S. Both devices were fabricated from the same batch.

Concentration of Na_2S	PCE_{max} [%]	V_{OC} [mV]	J_{SC} [mA/cm^2]	FF [%]	R_s [Ω·cm^2]	R_{sh} [Ω·cm^2]	G_{sh} [mS·cm^2]
0.1 M	12.74	491	39.3	66.0	0.51	1113	0.90
0.2 M	10.47	467	37.2	60.3	0.99	825	1.21

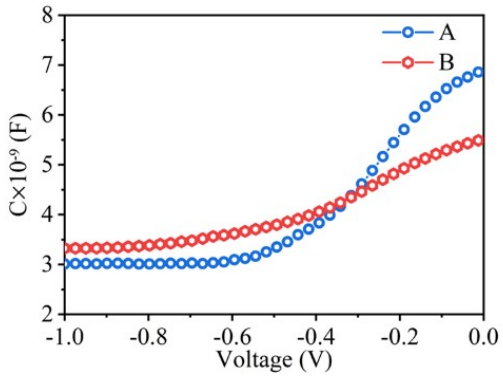

Figure S6. C-V curves of the champion device A and B.

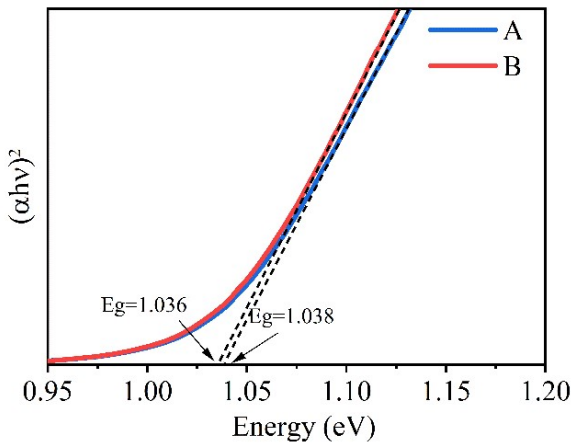

Figure S7. The optical band gap of the film A (1.036 eV) and B (1.038 eV) calculated from the UV–vis transmission spectra. The Na_2S layer spin-coated on the Mo substrate will not change the band gap of the CZTSSe absorbers.