

Supporting Information

Back contact interfacial modification mechanism in highly-efficient antimony selenide thin-film solar cells

Table S1. EDS results for Sb_2Se_3 thin films with different Mo substrates.

Sample	Sb (at. %)	Se (at. %)	Sb/Se ratio
S_{Mo1}	35.54	64.46	0.55
S_{Mo2}	38.09	61.91	0.62
S_{Mo3}	40.68	59.32	0.69

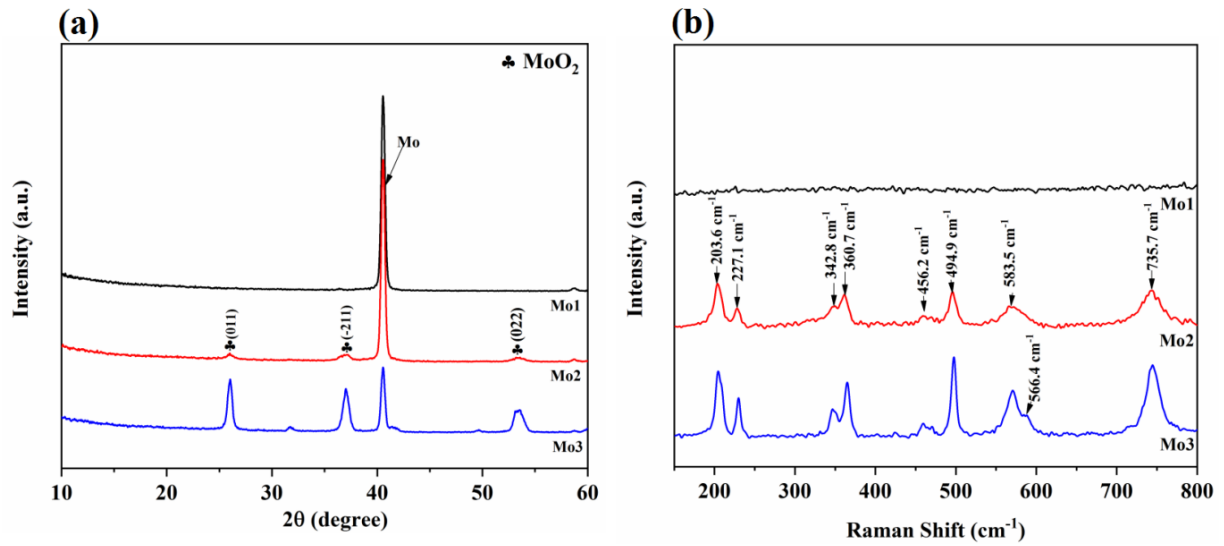


Fig. S1. (a) XRD patterns of Mo1, Mo2, and Mo3 substrates, and (b) Raman spectra of the surface of Mo1, Mo2, and Mo3 substrates.

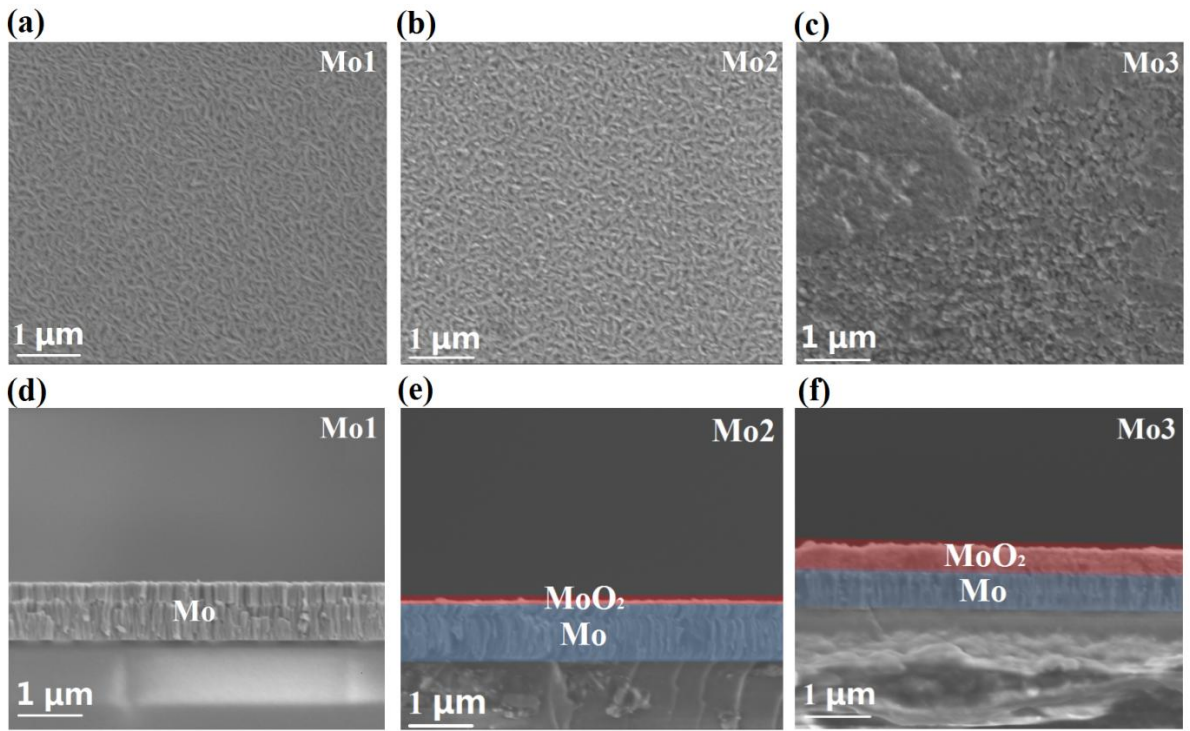
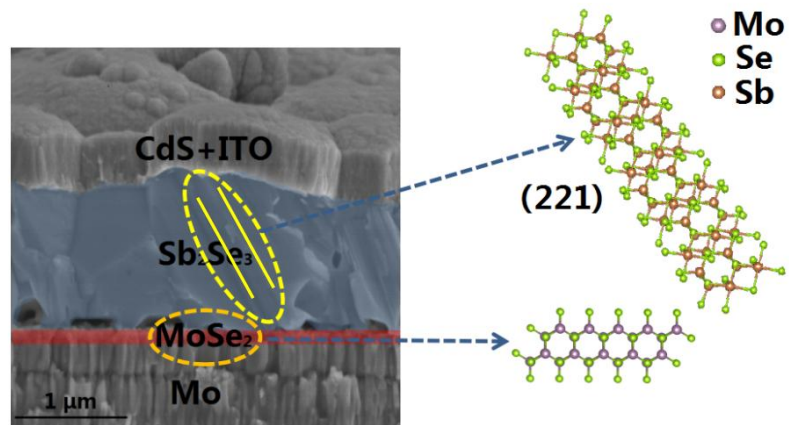


Fig. S2. (a-b) Surface SEM images of Mo substrates, and (d-f) cross-sectional SEM images of Mo substrates



WO- MoO₂ intermediate layer

Fig. S3. Cross-sectional SEM image of S_{Mo1} device (WO-MoO₂ intermediate layer)

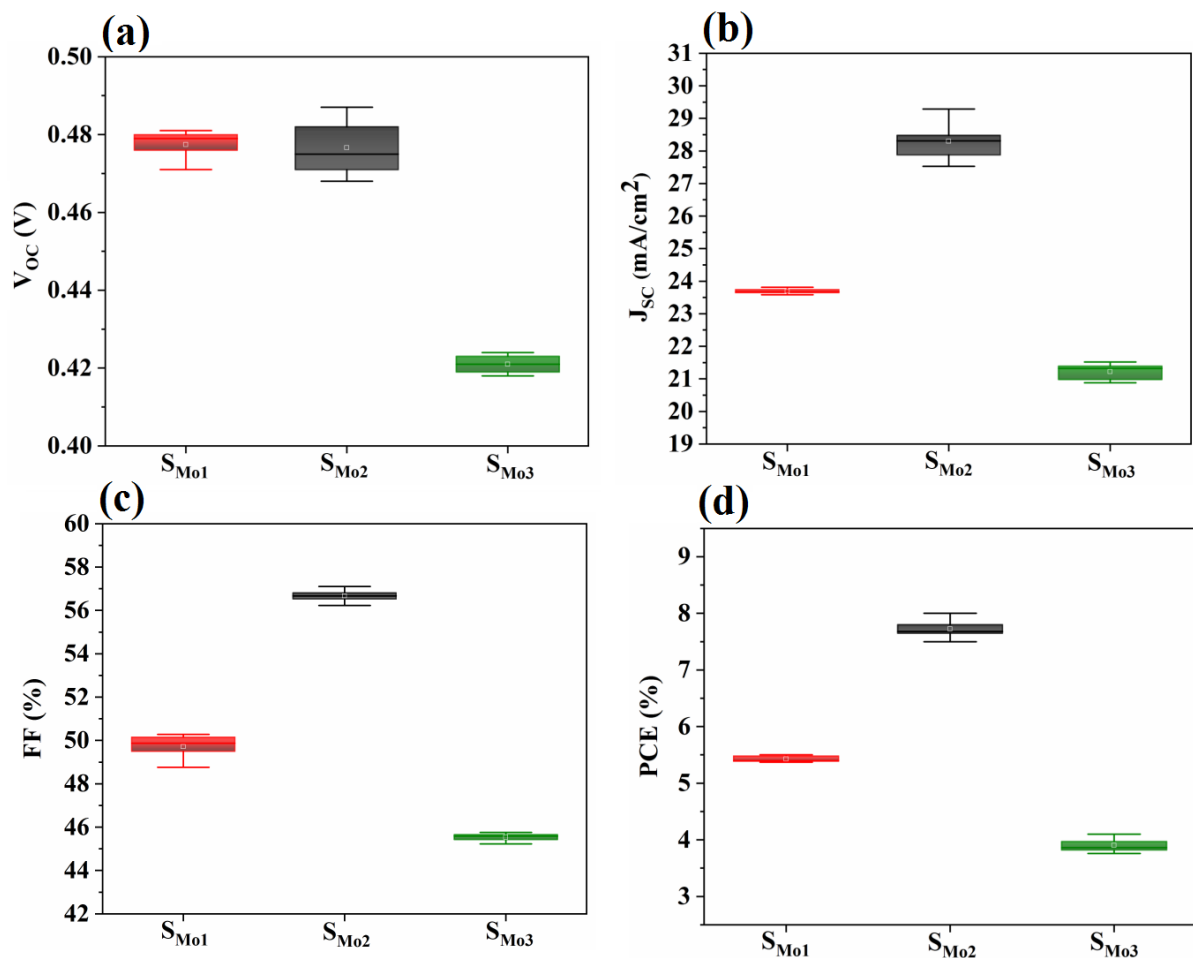


Fig. S4. Statistical distribution of the devices performance parameters including (a) open-circuit voltage (V_{OC}), (b) short-circuit current density (J_{SC}), (c) fill factor (FF), and (d) power conversion efficiency (PCE).

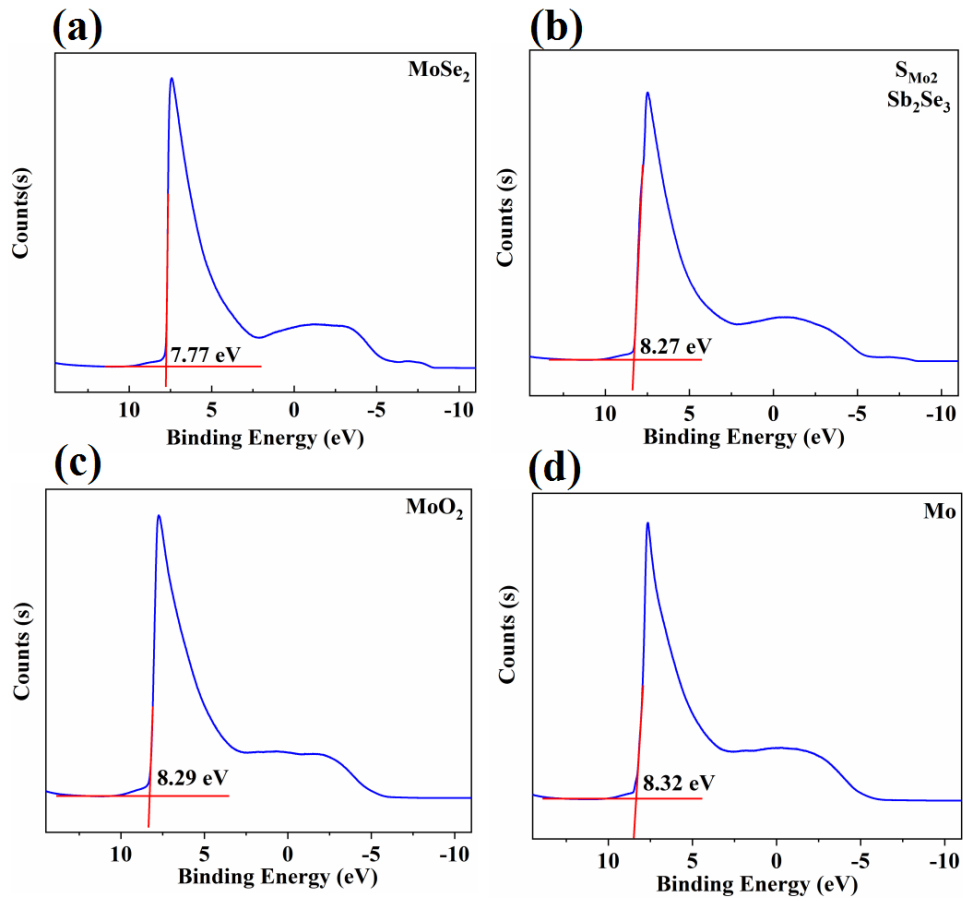


Fig. S5. UPS spectra for (a) the surface of MoSe₂ interface layer, (b) the back of Sb₂Se₃ layer in S_{Mo2} device, (c) the surface of MoO₂ intermediate layer, and (d) the surface of Mo.

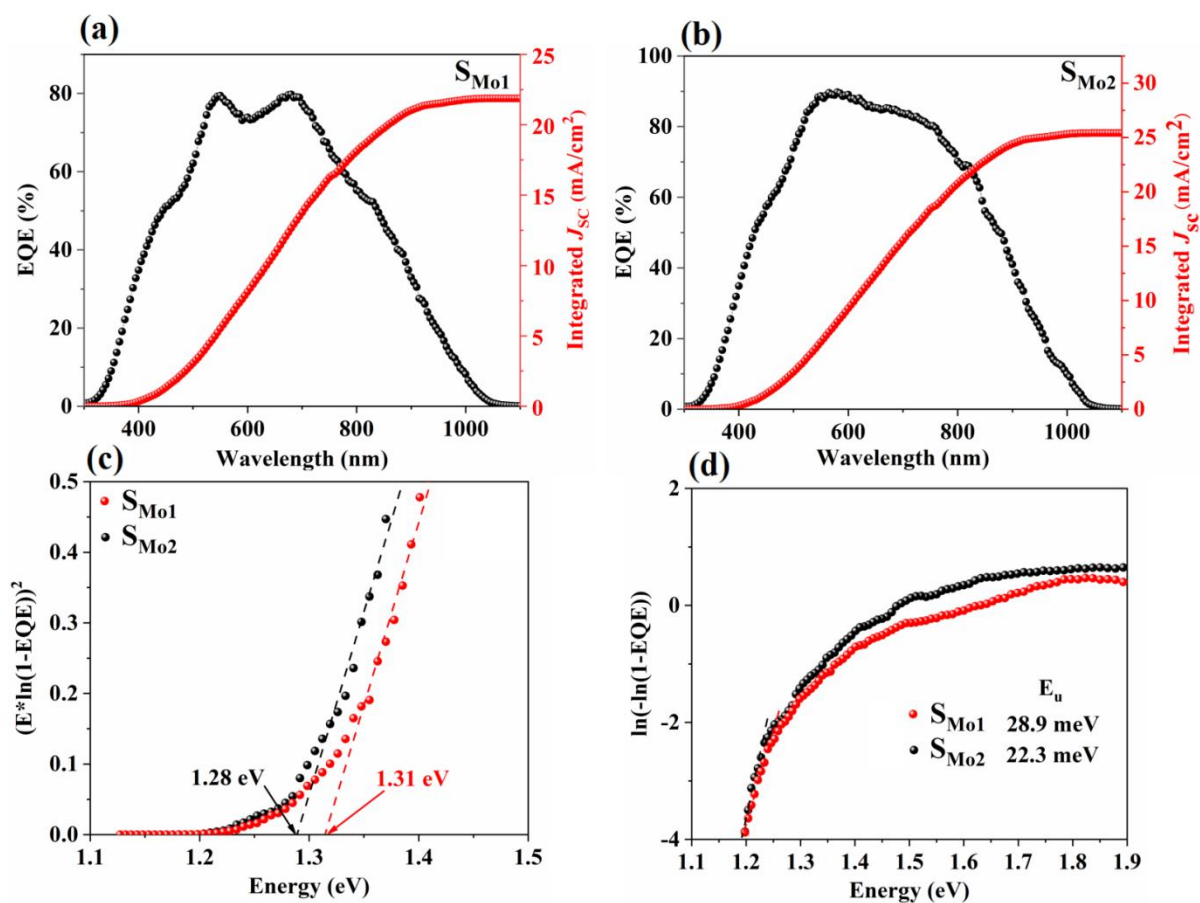


Fig. S6. (a) EQE and integrated J_{sc} of S_{Mo1} device, (b) EQE and integrated J_{sc} of S_{Mo2} device, (c) bandgap obtained from the EQE of solar cells, and (d) Urbach energy (E_u) obtained from the EQE of solar cells.

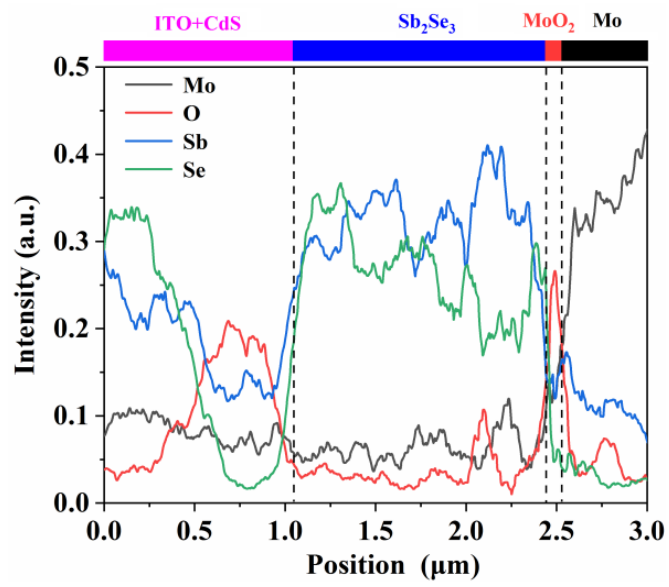


Fig. S7. EDS element depth profiles of Mo, O, Sb and Se elements in S_{Mo_2} device.

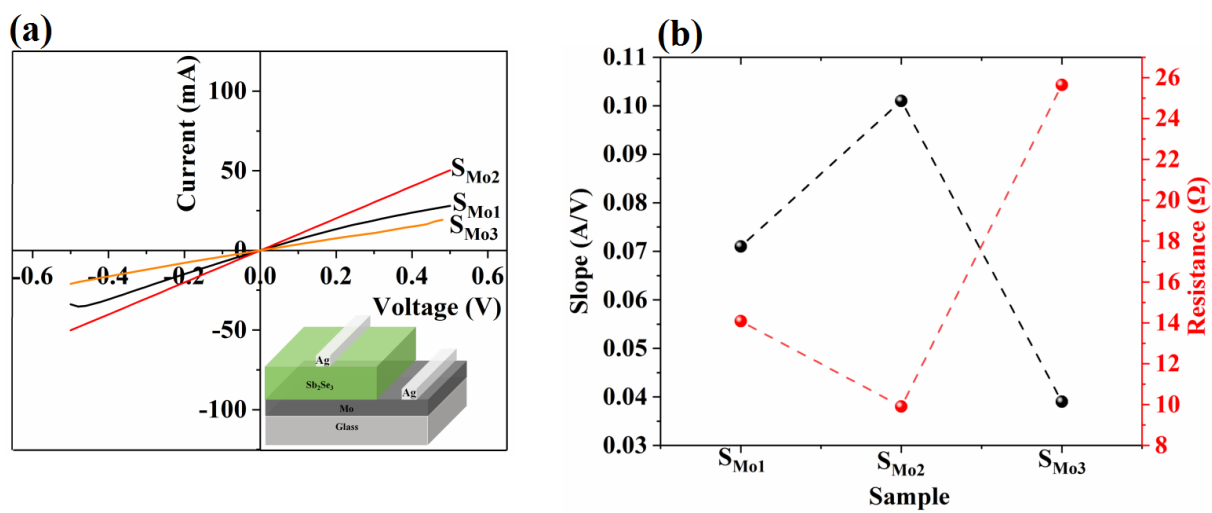


Figure S8. (a) I - V curves of Mo/ Sb_2Se_3 back contact (the schematic diagram of structure used to test I - V curves was inserted). (b) The slopes and resistance curves of S_{Mo1} , S_{Mo2} , and S_{Mo3} samples.