Supplementary Information for

Zn(O,S)-Based Electron-Selective Contacts with Tunable Band Structure for Silicon Heterojunction Solar Cells

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S1. Experimental Section

1. Preparation and characterization of Zn(O,S) films

Zn(O,S) films are deposited by radio frequency (RF) magnetron sputtering from a ceramic ZnS target (60 mm, diameter) in mixed working gas totally 0.8 Pa containing argon and oxygen with different proration (0 %, 0.3 %, 0.5 %, 0.7 %, 1.0 %) at a substrate temperature of 250 °C and an RF power of 100 W. By adjusting deposition time, ~10 nm and ~100 nm films are deposited on Schott glass and polished silicon which are given an ultrasonic cleaning prior to deposition. Transmission and reflection spectra of Zn(O,S) films (~100 nm) deposited on Schott glass are obtained with an Agilent cary 5000 UV-VIS-NIR spectrometer, and the optical bandgap E_g is fitted from the absorption spectrum listed in Table 1. XPS measurements are performed in a thermo fisher spectrometer with an Al monochromatic X-ray source. A He I ultraviolet source is used in UPS measurements. All measurements are performed on thin films (~10 nm) deposited on polished silicon. Keithley 6430 is used to measure the conductivity of Zn(O,S) films, as shown in Fig. 4a.

2. Device fabrication:

The solar cell (156 cm×156 cm) is fabricated on n-type CZ-Si wafers (1.0 Ω cm) with a thickness of ~180 μm. The textured front side with random pyramids has a boron diffused p+ emitter, which is passivated by SiN_x films. The front fingers are prepared by screen printing. All the processes mentioned above are completed in the production line to ensure the consistency of the process. The partially prepared solar cell is cut into a small size (1 cm×1 cm). The front side of the sample is well be protected before being given a short 5% HF etch. Then, the sample is rapidly transferred to the vacuum chamber. Zn(O,S) films are deposited at the rear of solar cells. Subsequently, the low-WF Mg metal layer (~7 nm) and the Ag electrode (1 μm) deposited by radio frequency (RF) magnetron sputtering covers on Zn(O,S) films.

3. Device characterization

The I–V characteristics of the solar cells are measured by using a Xenon-lamp solar simulator under standard 1 sun conditions (100 mW cm^{-2}, AM 1.5 spectrum, 25 °C), which is calibrated by a certified reference cell. The EQE spectrum of the solar cells is measured by employing a Zolix Corporation QE measurement system (Zolix solar cell scan 100). The pseudo light I-V curve is measured by Sinton Suns-V_{OC} illumination Voltage Tester at open circuit, so it is free from the effects of series

resistance. Suns-V_{oc} and pseudo-fill-factor can be extracted from the pseudo light I-V curve.

S2. Simulation detail

The software (AFORS-HET) is employed to simulate the energy band structure (in Fig. 7) and the photoelectric parameters of Zn(O,S)-based solar cells (in Fig. 8). The parameters of materials used in this study are listed in Table S1. To highlight the conduction-band offset impacts on the performance of solar cells, other parameters such as electron/hole mobility, donor concentration, conduction band effective density of states (N_c) and Valance band effective density of states (N_v) are assumed not subject to the composite of Zn(O,S) films.

Table S1. The simulation parameters of materials**.**

Parameters	n-c-Si	p^+-c-Si	Zn(O,S)
Thickness(nm)	2.0×10^5	3×10^2	10
Dielectric constant	11.9	11.9	10
Electron affinity (eV)	4.05	4.05	Variable
Band gap (eV)	1.12	1.12	Variable
Effective conduction band density (cm^{-3})	2.8×10^{19}	8.9×10^{18}	2.2×10^{18}
Effective valence band density (cm^{-3})	2.6×10^{19}	8.4×10^{18}	1.8×10^{19}
Electron mobility ($cm^2V^{-1}s^{-1}$)	1111	200	100
Hole mobility ($cm^2V^{-1}s^{-1}$)	421	77	25
Acceptor concentration (cm^{-3})	0	1×10^{19}	0
Donor concentration (cm^{-3})	1×10^{17}	0	1×10^{18}
Thermal velocity of electrons (cm/s)	1×10^7	1×10^7	1×10^5
Thermal velocity of hole (cm/s)	1×10^7	1×10^7	1×10^5
Layer density ($g.cm^{-3}$)	2.328	2.328	4.0

S3. Deposition rate

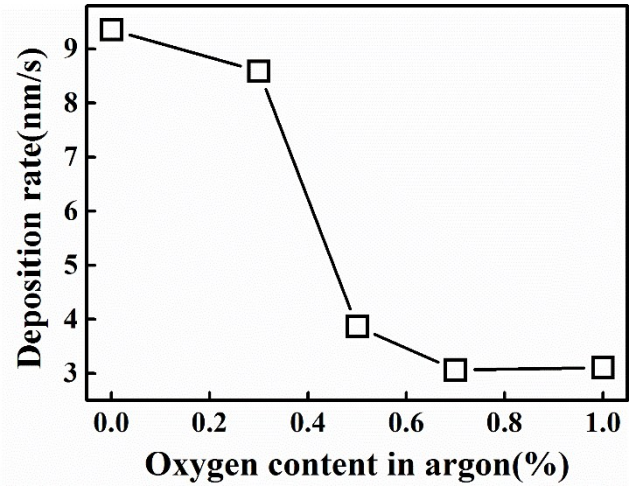

Fig. S1. Deposition rate varies with oxygen partial pressure (totally 0.8 Pa).

S4.Transmission and reflection spectra of Zn(O,S) films

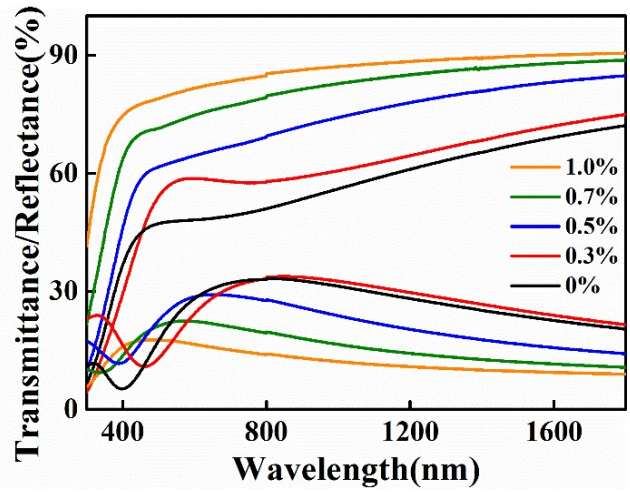

Fig. S2. Transmission and reflection spectra of Zn(O,S) films (~100 nm) deposited on schott glass. The desired thickness of Zn(O,S) films was deposited according to deposition rate by adjusting deposition time.

S5.Photovoltaic properties of p+/n-Si/Zn(O,S)/Ag heterojunction solar cells

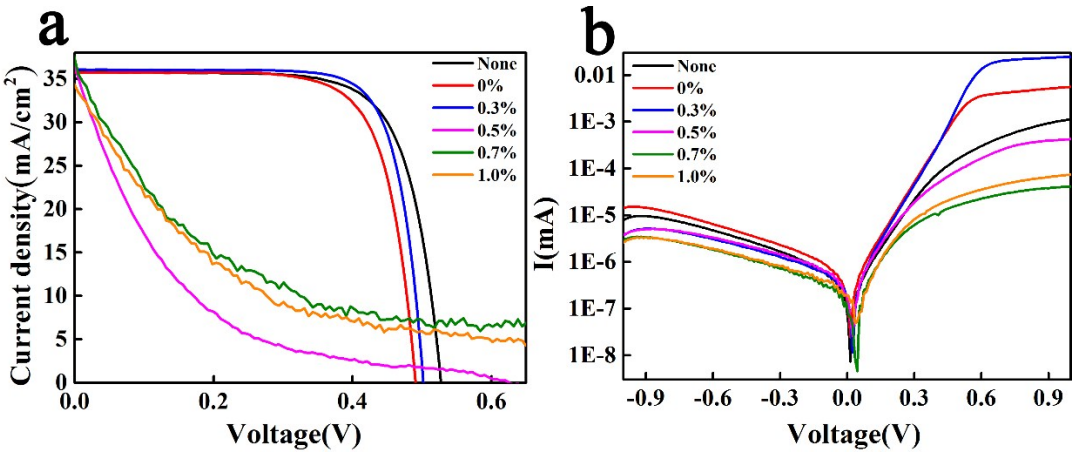

Fig. S3. The structure of n-type silicon solar cell featuring a full-area Zn(O,S)/Ag contact at the rear; (a) light J-V curves under AM 1.5 G;(b) log-plot dark I-V curves.

Table S2. Photovoltaic parameters of p+/n-Si/Zn(O,S)/Ag heterojunction solar cells

Dev.	O_2/Ar (%)	V_{oc} (mV)	J_{sc} (mA cm^{-2})	FF (%)	PCE (%)
1	None	511.6	35.9	74.4	13.7
2	0%	487.4	35.7	74.2	12.9
3	0.3%	500.0	36.1	77.3	14.0
4	0.5%	626.1	35.2	8.0	1.8
5	0.7%	975.9	35.6	13.4	4.7
6	1.0%	994.0	34.3	8.3	2.8