

BIFACIAL SOLAR CELL WITH SnS ABSORBER BY VAPOR TRANSPORT DEPOSITION

SUPPLEMENTARY INFORMATION

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SnS solar cell absorption calculations

In order to determine whether light absorption in the SnS layer was limiting the short-circuit current in our SnS-based solar cells, we performed diffuse reflectance and transmittance measurements using a Cary 6000 UV-Vis-NIR spectrophotometer (200 to 1800 nm) with an integrating sphere. As shown in Fig. S1, four material stacks were measured to isolate the fraction of incident light absorbed in the SnS layer as a function of wavelength, $A_{SnS}(\lambda)$.

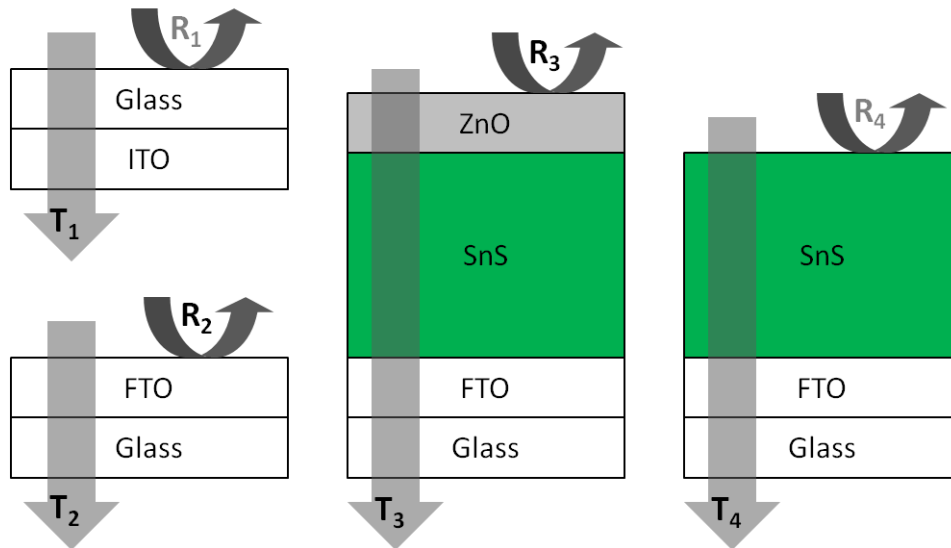


Figure S1: Diffuse reflectance and transmittance data from these four material stacks were used to estimate the fraction of incident light absorbed in the SnS layer.

Using the notation introduced in Fig. S1, the following equations can be established:

$$A_{SnS} = A_3 - A_2 - A_{ZnO}, \quad \text{[Equation S1a]}$$

$$A_3 = T_1(1 - T_3 - R_3), \quad \text{[Equation S1b]}$$

$$A_{ZnO} = T_1(1 - T_3/T_4 - R_3), \quad \text{[Equation S1c]}$$

$$A_2 = A_3 - T_1(1 - T_3/T_2 - R_3), \quad \text{[Equation S1d]}$$

where A , T , and R are wavelength dependent and represent percent absorption, transmittance and reflectance, respectively. This calculation assumes that the difference in reflection between SnS/air and SnS/ZnO as well as that between ZnO/air and ZnO/ITO are negligible.

To obtain the maximum short-circuit current (i.e. at 100% quantum efficiency), the product of absorption and the AM 1.5 G spectrum $G(\lambda)$ was integrated over all wavelengths above the SnS bandgap (1.0 eV) as follows:

$$J_{\max} = \int_{\lambda < 1240/m} G(\lambda) A_{SnS}(\lambda) d\lambda. \quad \text{[Equation S2]}$$

Using Eqn. S2, a maximum short-circuit current of 28 mA/cm² can be expected from our SnS-based solar cells if all the current is collected. For comparison, the maximum short-circuit current for a 1.0 eV bandgap material without optical losses is about 50 mA/cm².

Deposition methods

SnS by vapor transport deposition: The procedure for depositing SnS by vapor transport deposition [1] was modified to increase the deposition rate. In a three-zone horizontal tube furnace (Lindberg STF55666C), SnS powder was heated to 500 °C for 1.5 hours with flowing N₂ at 5 sccm and up to 100 mTorr. The substrate was placed 10 inches downstream at 365 °C. The pump used was a Leybold Trivac Model No. D8B (91255-1). The temperatures were calibrated with an external K-type thermocouple.

Mo by sputter deposition: Mo was sputtered at room temperature with 100 W DC power using a commercial sputter system (AJA International, Inc.). Either soda lime glass or single crystalline silicon was used as the substrate. The first layer was sputtered for 10 min at 10 mTorr of Ar

flowing at 6 sccm. The second layer was sputtered for 2 hours at 5.0 mTorr of Ar flowing at 6 sccm. The first high pressure layer is intended to control the stress in the film to prevent delamination. The second low pressure layer is intended to minimize the formation of interfacial material, which in the case of CIGS devices is MoSe_2 . A 2-inch diameter target (ACI Alloys, Inc.) was used.

ZnO by sputter deposition: ZnO was sputtered at room temperature with 80 W RF power for 1 hour in a 5 mTorr gas mixture consisting of Ar flowing at 15 sccm and O_2 flowing at 1 sccm. A commercial sputter system (AJA International, Inc.) was used with a 2-inch diameter target (ACI Alloys, Inc.).

ZnO by atomic layer deposition: Atomic layer deposition of ZnO was performed in a **GemStar 6 reactor (Arradiance Inc.)** using diethyl zinc and deionized water at 150 °C as precursors. The reactant exposure times were 30 ms for both precursors. N_2 was used to purge for 30 s in between exposures. 120 cycles were used.

Zn(O,S) by chemical bath deposition: In the same fashion as in Chapter 2, the Zn(O,S) bath was prepared by dissolving in deionized water the following: sodium citrate dihydrate (0.13 M), zinc acetate dihydrate (0.2 M), ammonium hydroxide (0.72 M), and thiourea (0.6 M). The substrate was mounted to the underside of a crystallization dish and immersed into the bath, which was maintained for 15 minutes at 70 °C using a jacketed beaker. Bubble formation on the substrate surface impedes growth uniformity and was thus removed by manual shaking.

TiO₂ by atomic layer deposition: Atomic layer deposition of TiO_2 was performed was performed in a **GemStar 6 reactor (Arradiance Inc.)** using titanium tetraisopropoxide and deionized water at 200 °C. The former was pulsed for 100 ms and purged for 20 seconds, while latter was pulsed for 2 seconds and purged for 60 seconds. 100 cycles were used.

CdS by chemical bath deposition: The CdS CBD bath was prepared by dissolving in deionized water the following: ammonium hydroxide (14.8 M), cadmium sulfate (0.015 M), thiourea (1.5 M). The substrate was mounted to the underside of a crystallization dish and immersed into the bath, which was maintained for 12 minutes at 65 °C using a jacketed beaker. Bubble formation on the substrate surface impedes growth uniformity and was thus removed by manual shaking.

ITO by sputter deposition: ITO was sputtered through a 0.01 cm^2 circularly patterned shadow mask at room temperature with 125 W RF power for 2 hours in a 2.5 mTorr gas mixture consisting for Ar flowing at 19 sccm and O_2 flowing at 1 sccm. The 2-inch diameter and 0.125 inch thick ITO target (ACI Alloys, Inc.) consisted of $\text{In}_2\text{O}_3/\text{SnO}_2$ by 90/10 weight percentage. A commercial sputter system (AJA International, Inc.) was used.

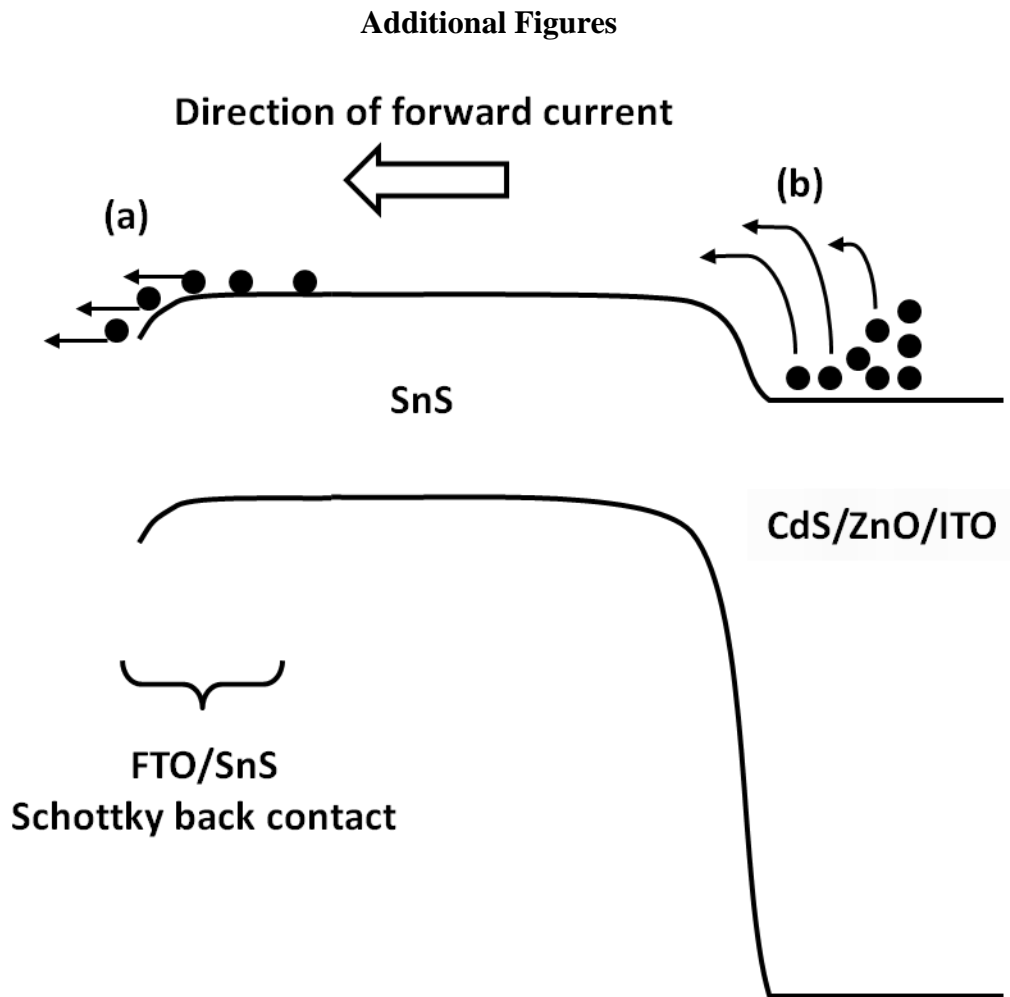


Figure S2: Hypothetical band diagram of a solar cell device stack consisting of glass/FTO/SnS/CdS/ZnO/ITO. In (a), photo-generated minority carrier electrons in the SnS conduction band are influenced by the hypothetical Schottky barrier to drift to the back contact, contributing to forward current. In (b), the energy gained by free-carrier absorption promotes forward current by helping electrons surmount the p-n junction

barrier. Backside illumination data indicates that the situation in (a) does not apply to the FTO/SnS interface. Figure made for conceptual purposes only and not drawn to scale.

References

[1] Wangperawong, A., Herron, S. M., Runser, R. R., Hägglund, C., Tanskanen, J. T., Clemens, B. M., & Bent, S. F. (2013). Vapor transport deposition and epitaxy of orthorhombic SnS on glass and NaCl substrates. *Applied Physics Letters*, *103*(5), 052105.