Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

Effects of bifunctional metal sulfide interlayers on photovoltaic properties of organic-inorganic hybrid solar cells

*B. Reeja-Jayan and Arumugam Manthiram**
Materials Science and Engineering Program
The University of Texas at Austin
Austin, Texas 78712, USA

1. SEM images of metal sulfide layers

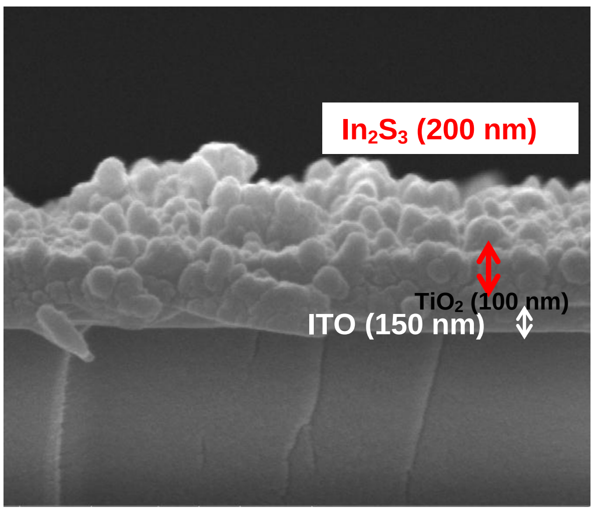

Fig. S1. Cross-sectional SEM image of In_2S_3 films (90 min) on TiO_2-coated ITO-glass substrates.

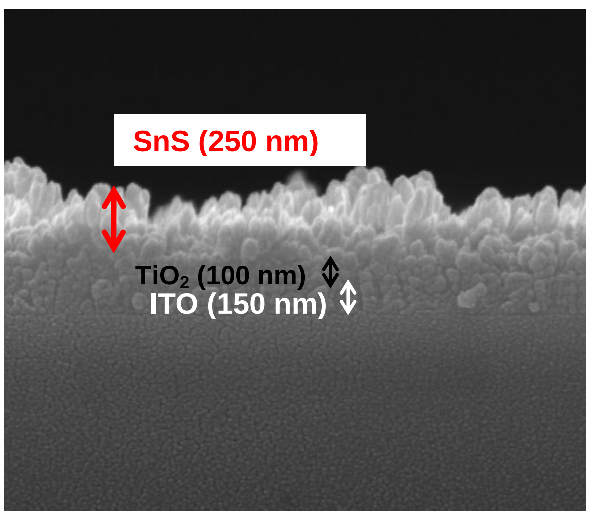

Fig. S2: Cross-sectional SEM image of SnS films (80 min) on TiO_2-coated ITO-glass substrates.

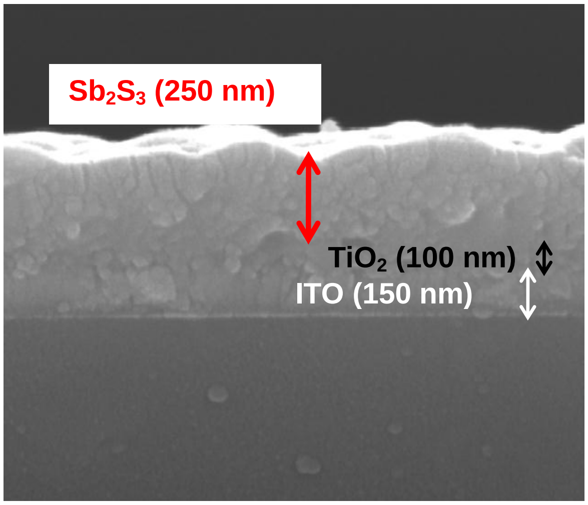

Fig. S3: Cross-sectional SEM image of Sb_2S_3 films (16 h) on TiO_2-coated ITO-glass substrates.

2. Determination of the absorption coefficient of metal sulfide layers

The absorption coefficient α (as a function of wavelength) was estimated using equation S1 [ref. 20 in the main manuscript]

$$\alpha = \frac{2.303\ \mathrm{Abs}}{t} \qquad \text{(S1)}$$

where, Abs is the measured absorbance (as a function of wavength) and t is the thickness of the metal sulfide film. For thickness calibration, the thickness t of all metal sulfide layers were ~ 250 nm. For background correction, the absorption spectra for the glass substrate, 150 nm thick ITO films and 100 nm thick TiO_2 films were obtained, and then subtracted from the metal sulfide spectra.

3. Determination of the band gap of metal sulfide layers

The direct energy bandgap was calculated using equation S2 [ref. 20 in the main manuscript]

$$(\alpha h\nu)^2 = A(E_g - h\nu) \qquad \text{(S2)}$$

The plot of $(\alpha h\nu)^2$ as a function of photon energy $h\nu$ is shown in Figure S4. The energy bandgap (E_g) was obtained by extrapolating the linear portion of this plot to intersect the energy ($h\nu$) axis.

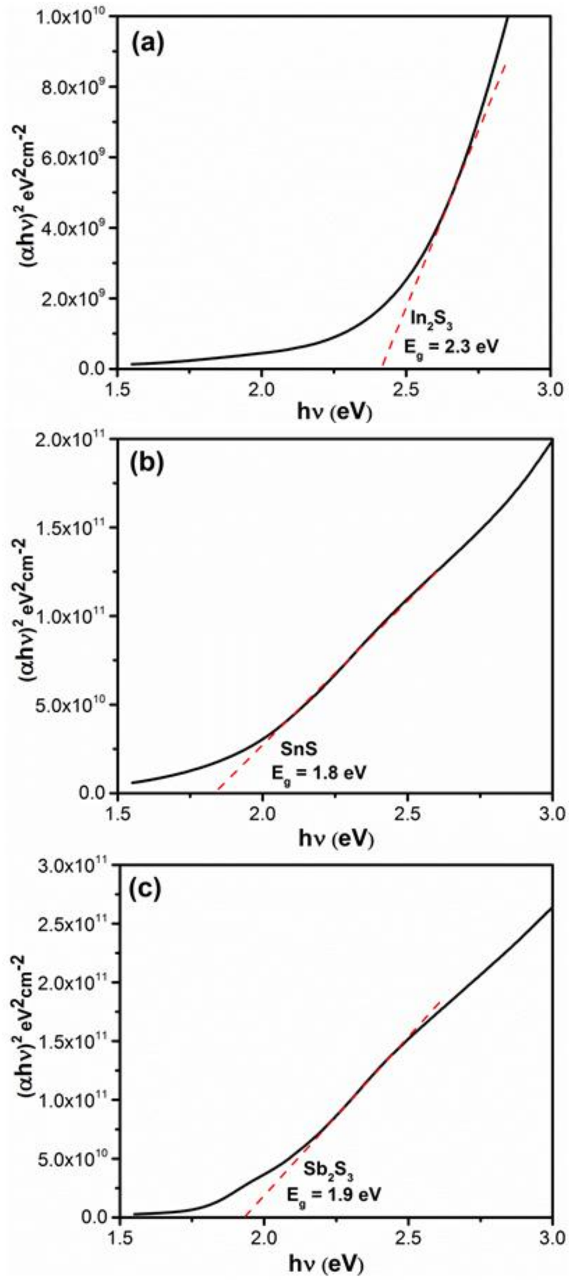

Fig. S4: Band gap calculation for (a) In_2S_3, (b) SnS, and (c) Sb_2S_3 metal films. TiO_2-coated ITO glass substrates were used as background reference, and their spectra were subtracted.

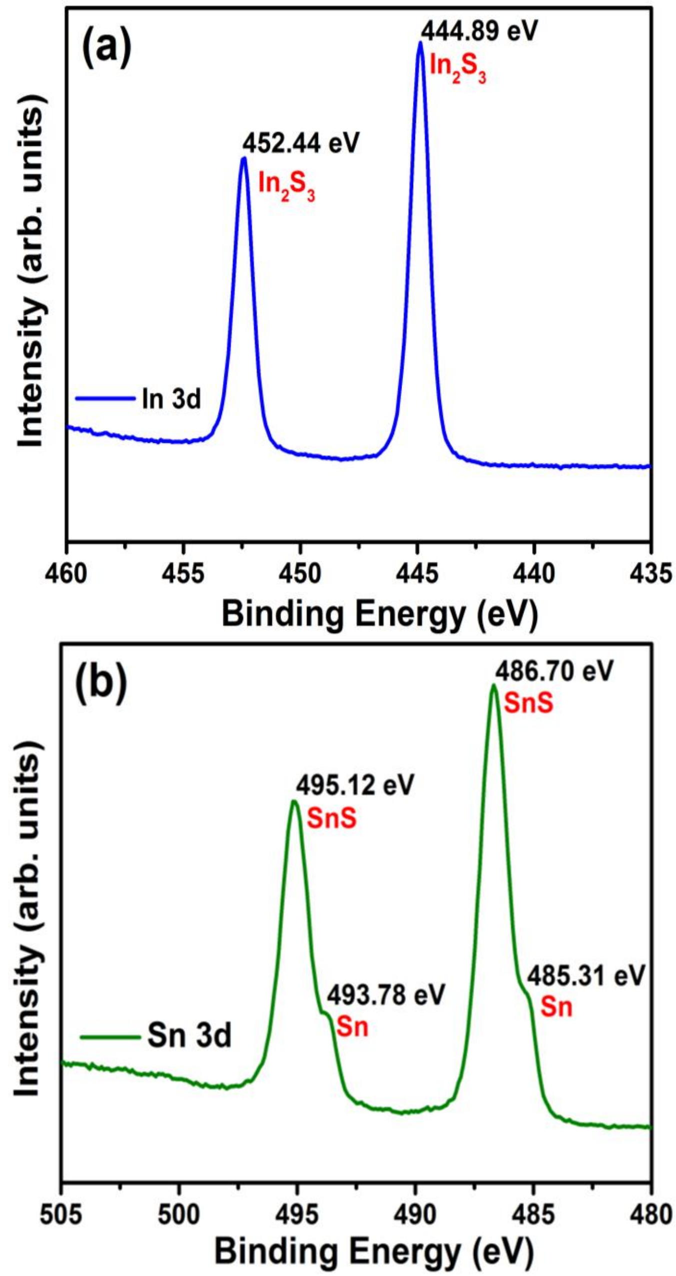

Fig. S5: XPS metal 3d spectra of (a) In and (b) Sn on surface of metal sulfides.