Supporting Information for

Scrutinizing the important roles of hole transport layers in near-intrinsic Sb_2S_3 planar solar cells

Qiang Xie,[1] Jiacheng Zhou,[1] Wenfei Wei,[2] Naiqiang Yin,*[,3] and Ru Zhou*[,1]

[1] School of Electrical Engineering and Automation, Hefei University of Technology, Hefei 230009, P. R. China

[2] School of Physics, Hefei University of Technology, Hefei 230009, P. R. China

[3] School of Physics and Electronic Engineering, Qilu Normal University, Jinan 250200, China

* Corresponding authors:

yinnq@foxmail.com (Naiqiang Yin)

zhouru@hfut.edu.cn (Ru Zhou)

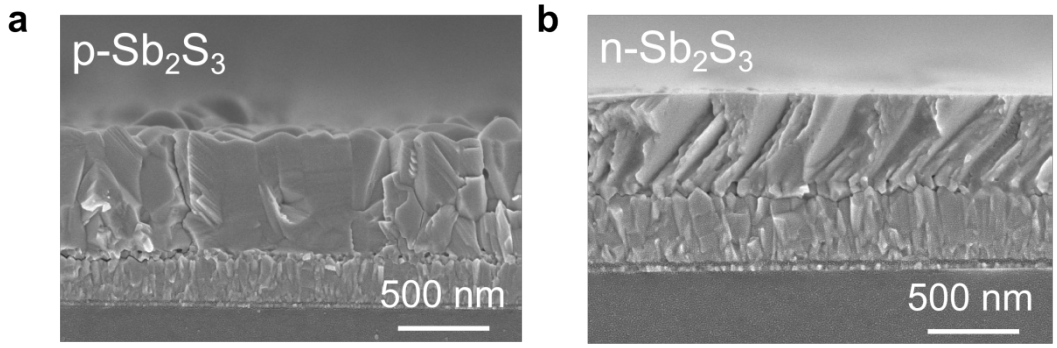

Fig. S1. (Color online) Cross-sectional-view SEM images of (a) p-type and (b) n-type Sb_2S_3 thin films.

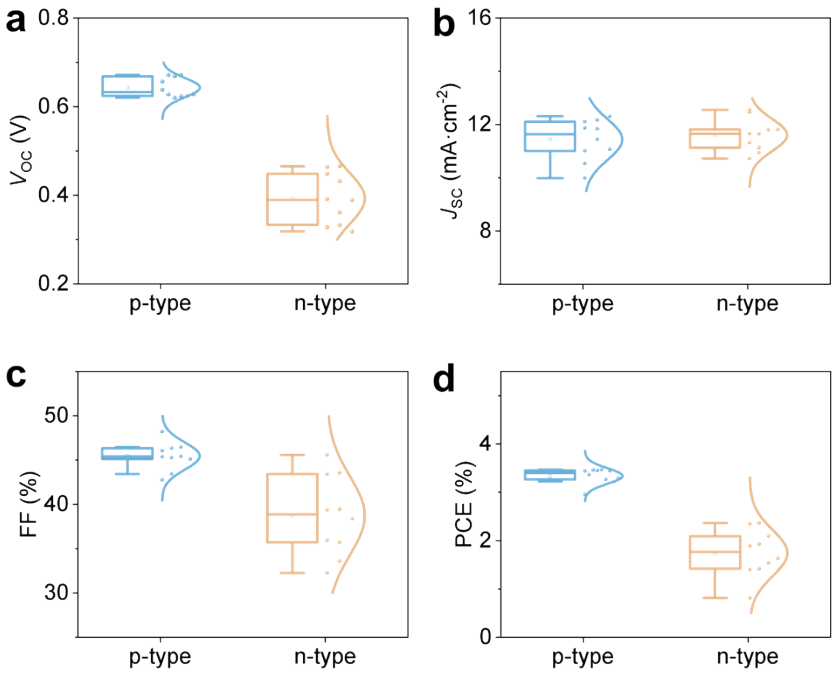

Fig. S2. (Color online) Statistics of performance parameters of FTO/CdS/p-Sb_2S_3/Au and FTO/CdS/n-Sb_2S_3/Au solar cells: (a) V_{OC}, (b) J_{SC}, (c) FF, (d) PCE.

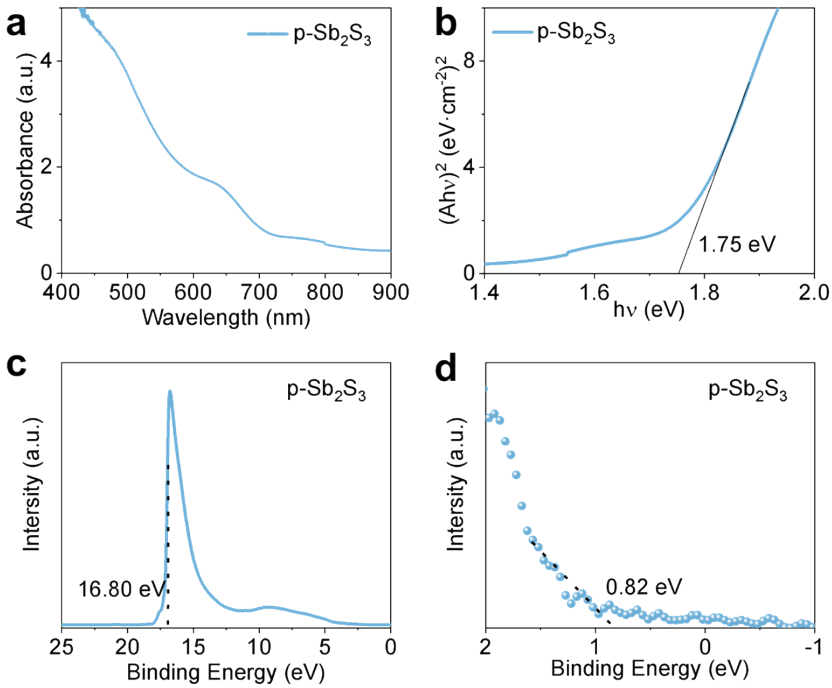

Fig. S3. (Color online) (a)-(b) Absorption spectrum and Tauc plots for p-Sb_2S_3 films. UPS spectrum of p-Sb_2S_3 near (c) the secondary electron cutoff edge and (d) the Fermi edge.

Table S1. Photovoltaic performance parameters of FTO/CdS/Sb_2S_3/Au and FTO/CdS/Sb_2S_3/Spiro-MeTAD/Au based on SCAPS simulations.

Device	V_{OC} (V)	J_{SC} (mA·cm^{-2})	FF (%)	PCE (%)
FTO/CdS/p-Sb_2S_3/Au	1.02	19.62	68.69	13.78
FTO/CdS/p-Sb_2S_3/Spiro-OMeTAD/Au	1.09	19.72	78.85	16.89
FTO/CdS/n-Sb_2S_3/Au	0.82	18.75	83.48	12.84
FTO/CdS/n-Sb_2S_3/Spiro-OMeTAD/Au	1.29	18.84	84.79	20.66

Table S2. Basic material parameters of different HTLs

Parameter	Cu_2O	CuSCN	CuI	Spiro-OMeTAD
Thickness (nm)	200	200	200	200
Dielectric permittivity	7.11	10	6.5	3
Bandgap, E_g (eV)	2.17	3.6	2.98	3.17
Electron affinity, χ (eV)	3.2	1.7	2.1	2.05
Electron mobility (cm^2·V^{-1}·s^{-1})	200	100	1.7×10^{-4}	2×10^{-4}
Hole mobility (cm^2·V^{-1}·s^{-1})	80	25	2×10^{-4}	2×10^{-4}
CB effective density of states (cm^{-3})	2.02×10^{17}	2.2×10^{19}	2.8×10^{19}	2.2×10^{18}
VB effective density of states (cm^{-3})	1.1×10^{19}	1.8×10^{19}	10^{19}	1.8×10^{19}
Acceptor doping concentration (cm^{-3})	2×10^{19}	2×10^{19}	2×10^{19}	2×10^{19}
Donor doping concentration (cm^{-3})	-	-	-	-
Electron/hole thermal velocity (cm^{-3})	10^7	10^7	10^7	10^7
Defect density (cm^{-3})	10^{15}	10^{15}	10^{15}	10^{15}