Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information:

Multiple states and roles of hydrogen in *p*-type SnS semiconductor

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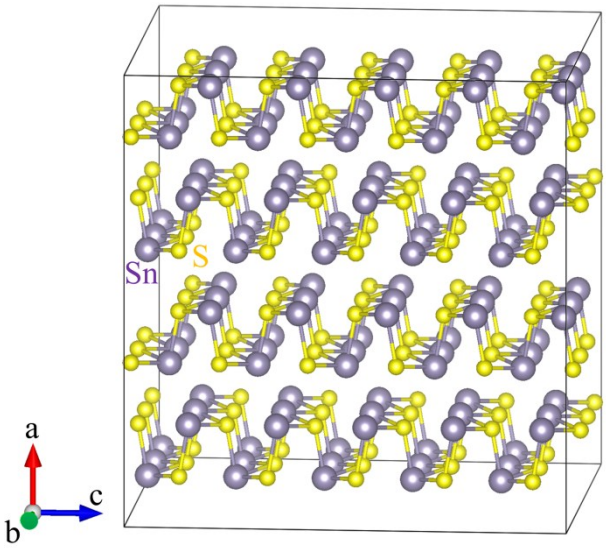

Fig. S1 400-atoms supercell (5×5×2 unit cells) used for modeling defects and impurities in SnS.

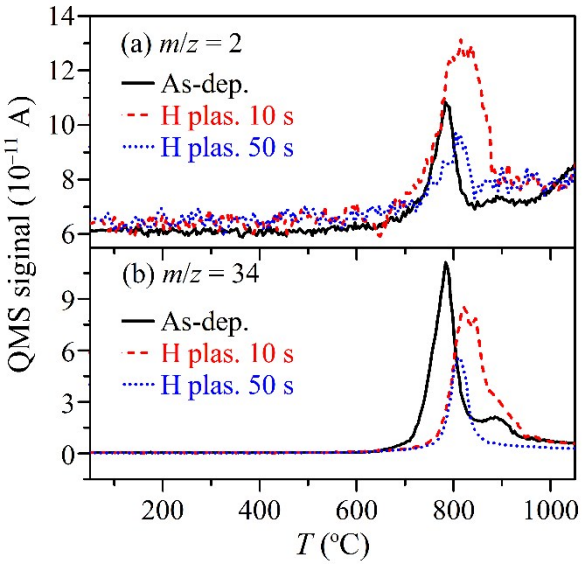

Fig. S2 TDS spectra for (a) $m/z = 2$ (corresponding to H_2) and (b) $m/z = 34$ (corresponding to H_2S) for as-deposited and H plasma exposed SnS films.

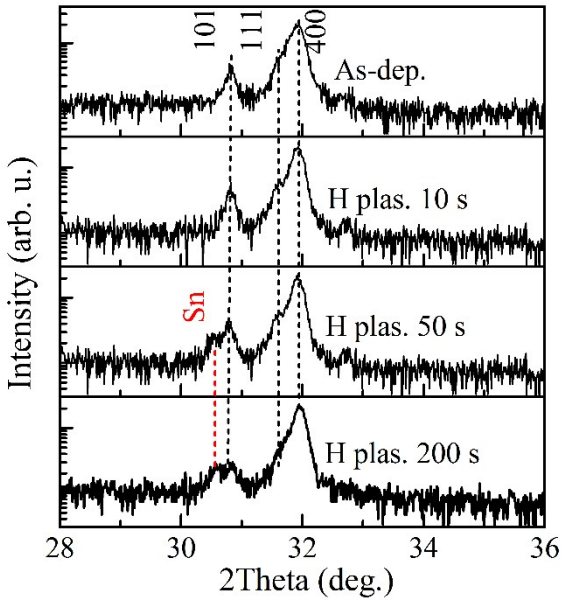

Fig. S3 XRD patterns of as-deposited and H plasma treated SnS films. The diffraction peak from Sn metal is indicated by the red vertical line.

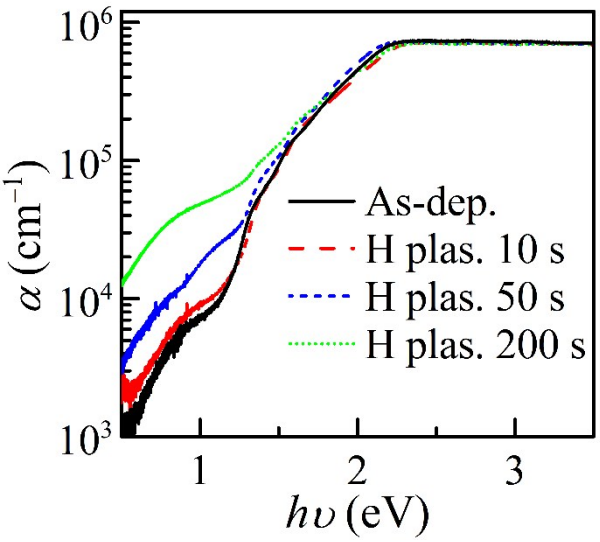

Fig. S4 Optical absorption spectra of as-deposited and H plasma treated SnS films.

Table S1. Calculated formation enthalpies (ΔH in eV) of neutral intrinsic defects and H-related impurities.

	V_{Sn}	V_S	Sn_i	S_i	Sn_S	S_{Sn}	H_i	H_{Sn}	$[2H]_{Sn}$	$[3H]_{Sn}$	H_S	$[2H]_S$	$[3H]_S$
Sn-poor	1.33	1.76	3.27	1.40	2.88	2.27	1.29	0.73	0.30	1.22	2.37	2.02	2.89
Sn-rich	2.01	1.08	2.59	2.09	1.51	3.64	1.29	1.41	0.98	1.90	1.68	1.33	2.20