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

Supplementary material for "First principles study of point defects in SnS"

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I. LOCAL STRUCTURES SURROUNDING THE RELAXED DEFECTS

In order to assist in future computational models and to assist in the experimental identification of the defects studied in this work, we provide in Table I and Table II the neighbor bond lengths surrounding each extrinsic defect (up to a cutoff of 3.5 Å). These bond lengths respresent the structures as relaxed within DFT using the PBE functional (as discussed in the main body).

TABLE I. Neighboring atomic environment for the extrinsic defects As, Cd, Cl, Cu, In, and Mo, all in their neutral charge state. For each defect, the bond lengths of the closest atoms within a 3.5 Å cutoff from the defect site are given.

Defect	Sn neighbors (Å)	S neighbors (Å)
As_i	2.72, 2.89, 2.94	2.24, 2.91
As_{Sn}	—	2.32, 2.34, 2.34, 3.48, 3.48
As_S	2.76, 2.77, 2.77, 3.20, 3.20, 3.21	—
Cd_i	2.73, 2.85, 3.47	2.55, 2.64
Cd_{Sn}	—	2.53, 2.53, 2.53
Cd_S	2.93, 3.00, 3.00, 3.17, 3.17, 3.37	—
Cl_i	2.42, 3.09, 3.10	3.23, 3.24, 3.39, 3.42
Cl_{Sn}	2.77, 2.77	3.29, 3.29, 3.33, 3.45, 3.48, 3.48, 3.49
Cl_S	2.90, 2.90, 2.99	—
Cu_i	2.63, 2.64, 3.09, 3.36	2.24, 2.24, 3.32
Cu_{Sn}	3.28, 3.28	2.25, 2.25, 2.26
Cu_S	2.70, 2.70, 2.70, 2.92, 2.92, 3.07	—
In_i	2.90, 2.95, 3.27	2.63, 2.68, 3.12
In_{Sn}	—	2.62, 2.67, 2.67, 3.32, 3.32
In_S	2.95, 2.95, 2.98, 3.25, 3.25, 3.38	
Mo_i	2.68, 2.72, 2.93, 2.99	2.36, 2.41, 2.61
Mo_{Sn}	—	2.44, 2.44, 2.49, 2.59
Mo_S	2.68, 2.79, 2.79, 2.95, 2.95, 3.18	2.63, 2.63

TABLE II. Neighboring atomic environment for the extrinsic defects N, Na, O, P, Sb, and Zn, all in their neutral charge state. For each defect, the bond lengths of the closest atoms within a 3.5 Å cutoff from the defect site are given.

Defect	Sn neighbors (Å)	S neighbors (Å)
N_i	1.99, 2.10, 3.19	2.66, 3.23, 3.47
N_{Sn}	3.16, 3.16	2.54, 2.66, 2.66
N_S	2.14, 2.17, 2.17	3.47, 3.47
Na_i	2.92, 2.97, 3.19, 3.21	2.54, 2.62, 2.63
Na_{Sn}	—	2.80, 2.83, 2.83, 3.31, 3.31, 3.45
Na_S	3.00, 3.14, 3.14, 3.39	2.94, 2.94
O_i	1.96, 2.33, 2.34	2.94, 3.21, 3.23, 3.23
O_{Sn}	2.58, 2.58	2.36, 2.36, 2.99
O_S	2.20, 2.22, 2.22	3.35, 3.35
P_i	2.63, 2.80, 2.82	2.07, 3.01
P_{Sn}	—	2.17, 2.18, 2.18
P_S	2.65, 2.67, 2.67, 3.17, 3.17, 3.20	—
Sb_i	2.88, 3.06, 3.30, 3.41, 3.46	2.48, 2.85
Sb_{Sn}	—	2.52, 2.55, 2.55, 3.38, 3.38
Sb_S	2.94, 2.94, 2.95, 3.27, 3.27, 3.27	—
Zn_i	2.60, 2.77	2.35, 2.41
Zn_{Sn}	3.42, 3.43	2.29, 2.29, 2.29
Zn_S	2.80, 2.80, 2.80, 3.15, 3.15, 3.40	—