Unraveling the enhancement mechanisms of H_2S sensing in SnO_2 surface: an *ab initio* perspective

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Table S1 Some concerned Sn(Sb)-O bond lengths in SnO_2 before and after Sb-doping.

Bond (Å)	Sn_{6c}-O_b	Sn_{6c}-O_p	Sn_{5c}-O_p	Sn_{5c}-O_{3b}
SnO_2(110)	1.966	2.107	2.029	1.971
Sb_{5c6c}/SnO_2(110)	1.963	2.039	2.181	2.207

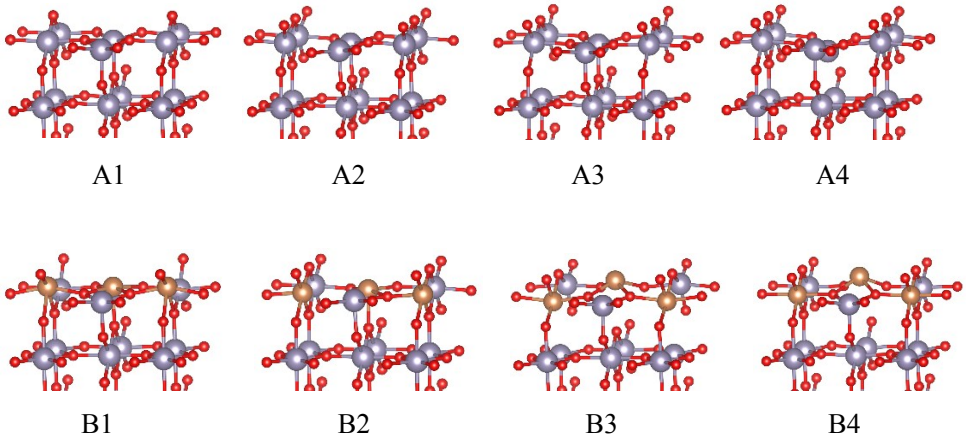
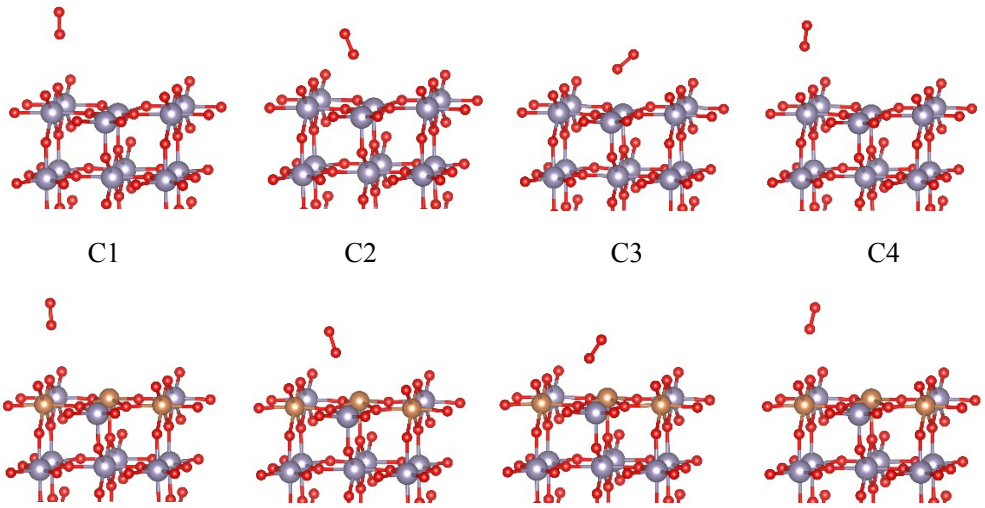


Fig. S1 Optimized surface of SnO_2(110) and Sb_{5c6c}/SnO_2(110) with various oxygen defects. (A1; B1) skin layer bridging oxygen; (A2; B2) skin layer plane oxygen; (A3; B3) inner layer the first bridging oxygen; (A4; B4) inner layer the second bridging oxygen.

Table S2 The adsorption energy (eV) of O_2 at different positions on the surface of SnO_2(110) and Sb_{5c6c}/SnO_2(110).

Adsorption sites	O_b	O_p	Sn_{5c}	Sn_{6c}	Sb_{5c}	Sb_{6c}
SnO_2(110)	-0.0512	-0.1474	-0.2575	-0.0703	-	-
Sb_{5c6c}/SnO_2(110)	-0.0509	-0.1270	-0.1901	-0.0637	-0.0795	-0.0564



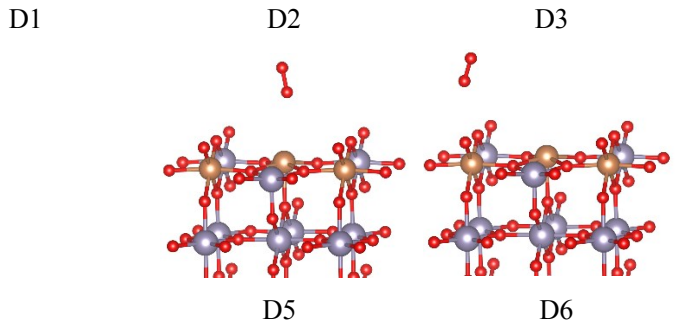


Fig. S2 Optimized adsorption structure of O_2 on SnO_2 (110) and Sb_{5c6c}/SnO_2 (110) surface at different positions. (C1-C4) O_2 molecular is adsorbed respectively at the sites of O_b; O_p; Sn_{5c} and Sn_{6c} on the SnO_2(110) surfaces. (D1-D6) O_2 molecular is adsorbed respectively at the sites of O_b; O_p; Sn_{5c}; Sn_{6c}; Sb_{5c} and Sb_{6c} on the Sb_{5c6c}/SnO_2(110) surfaces.

Table S3 The dissociative O^- atom adsorption energy (eV) at different positions on the surface of SnO_2(110) and Sb_{5c6c}/SnO_2.

Adsorption sites	O_b	O_p	Sn_{5c}	Sn_{6c}	Sb_{5c}	Sb_{6c}
SnO_2(110)	2.7858	1.3996	1.4172	2.7859	-	-
Sb_{5c6c}/SnO_2(110)	2.8527	0.2391	0.9195	1.5265	0.0627	2.8428

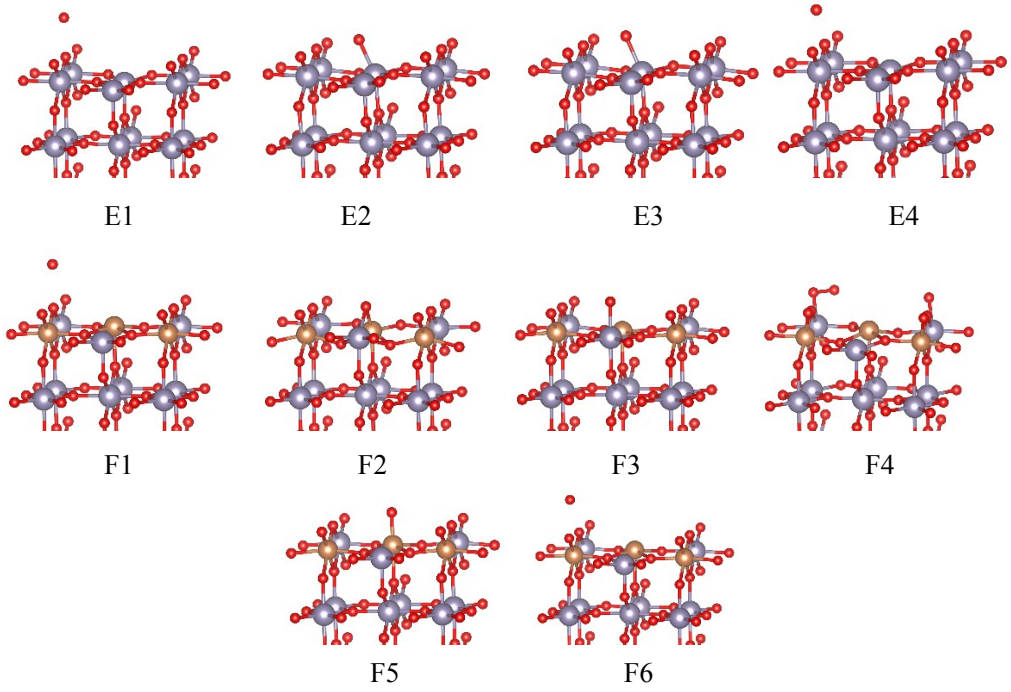


Fig. S3 Optimized structure of dissociative O^- atom absorption at different positions on the surface of SnO_2(110) and Sb_{5c6c}/SnO_2(110). (E1-E4) O atom is adsorbed respectively at the sites of O_b; O_p; Sn_{5c} and Sn_{6c} on the SnO_2(110) surfaces. (F1-F6) O atom is adsorbed respectively at the sites of O_b; O_p; Sn_{5c}; Sn_{6c}; Sb_{5c} and Sb_{6c} on the Sb-doped SnO_2(110) surfaces.

Table S4 The adsorption energy (eV) of O_2 at different positions on the surface of Sb-doped SnO_2(110) with O_b vacancy($V(O_b)$). V(o)1 represents that O_2 is placed above the oxygen vacancy and parallel to the X axis. V(o)2 means that O_2 is placed above the oxygen vacancy and parallel to the Y axis.

Adsorption sites	O_b	O_p	Sn_{5c}	Sn_{6c}	Sb_{5c}	Sb_{6c}	V(o)1	V(o)2
Sb_{5c6c}/SnO_2(110)	-1.1461	-0.1217	-0.1471	-0.1066	-0.1056	-0.0899	-1.3710	-1.2153

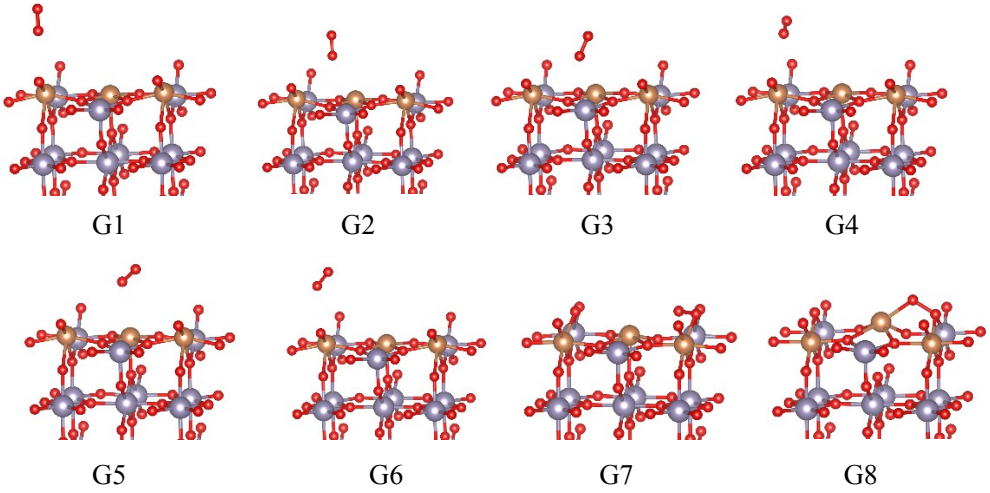
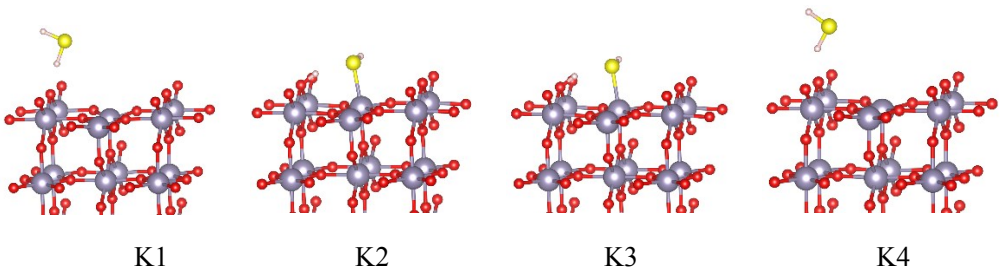


Fig. S4 Optimized adsorption structure of O_2 on Sb_{5c+6c}/SnO_2 (110) surface with O_b vacancy at different positions. (G1-G6) O_2 molecular adsorption respectively at the sites of O_b ; O_p; Sn_{5c}; Sn_{6c}; Sb_{5c}; Sb_{6c}. (G7) O_2 molecular is placed above the oxygen vacancy and parallel to the X axis. (G8) O_2 molecular is placed above the oxygen vacancy and parallel to the Y axis.

Table S5 The adsorption energy (eV) of H_2S at different positions on the surface of SnO_2(110) and Sb-doped SnO_2(110).

Adsorption sites	O_b	O_p	Sn_{5c}	Sn_{6c}	Sb_{5c}	Sb_{6c}
SnO_2(110)	-0.2809	-2.0670	-2.0749	-0.1984	-	-
Sb_{5c6c}/SnO_2(110)	-0.1629	-1.5819	-1.5921	-0.2337	-0.1158	-0.1861



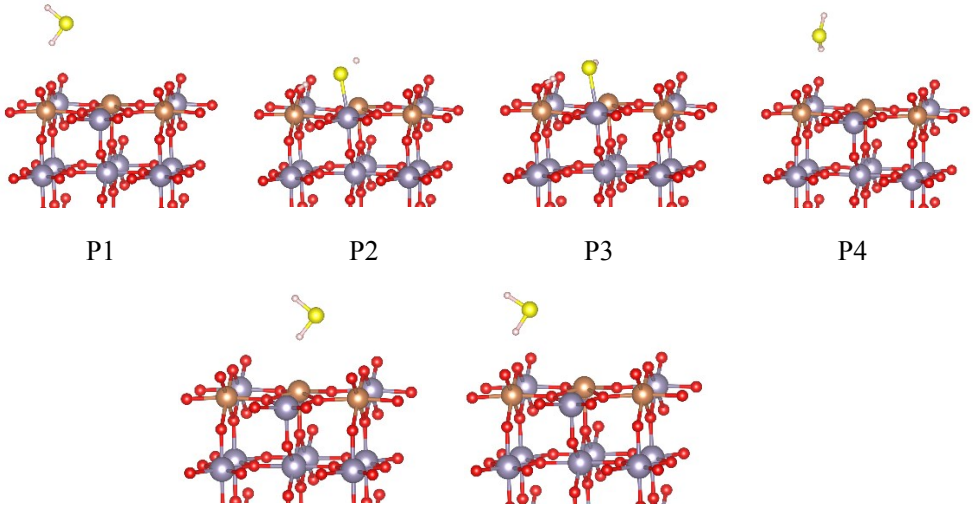


Fig. S5 Optimized structure of H_2S at different positions on the surface of $SnO_2(110)$ and $Sb_{5c6c}/SnO_2(110)$. (K1-K4) H_2S molecular is adsorbed respectively at the sites of O_b; O_p; Sn_{5c} and Sn_{6c} on the $SnO_2(110)$ surfaces. (P1-P6) H_2S molecular is adsorbed respectively at the sites of O_b; O_p; Sn_{5c}; Sn_{6c}; Sb_{5c} and Sb_{6c} on the $Sb_{5c6c}/SnO_2(110)$ surfaces.

Table S6 The adsorption energy (eV) of H_2S at different positions on the surface of Sb-doped $SnO_2(110)$ with O_b vacancy.

Adsorption sites	O_b	O_p	Sn_{5c}	Sn_{6c}	Sb_{5c}	Sb_{6c}	V(o)
$Sb_{5c6c}/SnO_2(110)$	-0.1214	-0.2163	-1.5280	-0.3819	-0.1921	-0.2636	-0.3746

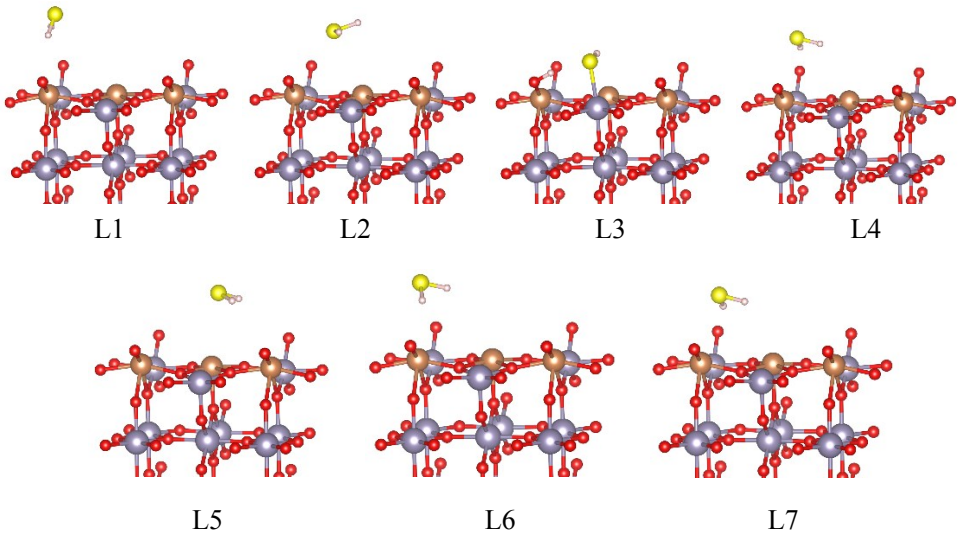


Fig. S6 Optimized structure of H_2S at different positions on the surface of $Sb_{5c6c}/SnO_2(110)$ with O_b vacancy. (L1-L6) H_2S molecular is adsorbed respectively at the sites of O_b; O_p; Sn_{5c}; Sn_{6c}; Sb_{5c} and Sb_{6c} on the $Sb_{5c6c}/SnO_2(110)$ surfaces. (L7) H_2S molecular is adsorbed at the sites of O_b vacancy.

Table S7 The adsorption energy (eV) of H_2S at different positions on the surface of Sb-doped $SnO_2(110)$ with pre-adsorbed O_2^-.

Adsorption sites	O_b	O_p	Sn_{5c}	Sn_{6c}	Sb_{5c}	Sb_{6c}
$Sb_{5c6c}/SnO_2(110)$	-0.1957	-1.6601	-1.1299	0.0577	-0.3271	-0.9727

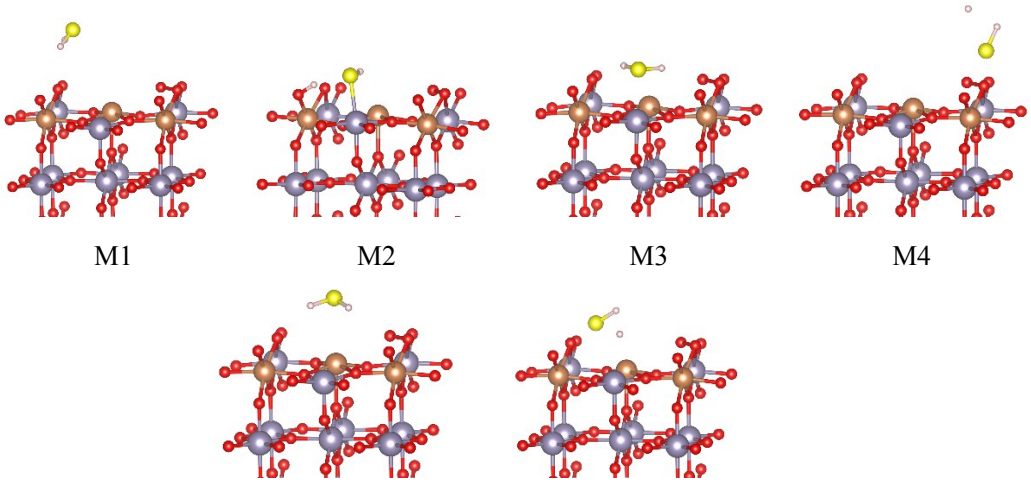


Fig. S7 Optimized structure of H_2S at different positions on the surface of $Sb_{5c6c}/SnO_2(110)$ with pre-adsorbed O_2^-. (M1-M6) H_2S molecular is adsorbed respectively at the sites of O_b; O_p; Sn_{5c}; Sn_{6c}; Sb_{5c} and Sb_{6c} on the surface.

Table S8 The adsorption energy (eV) of H_2S at different positions on the surface of Sb-doped $SnO_2(110)$ with preadsorbed O^-. note: $O(Sb_{5c})$ represents O adsorbed on Sb_{5c}.

Adsorption sites	O_b	O_p	Sn_{5c}	Sn_{6c}	$O(Sb_{5c})$	Sb_{6c}
$Sb_{5c6c}/SnO_2(110)$	-0.2744	-3.1022	-3.1183	-0.5022	-0.3168	-0.4842

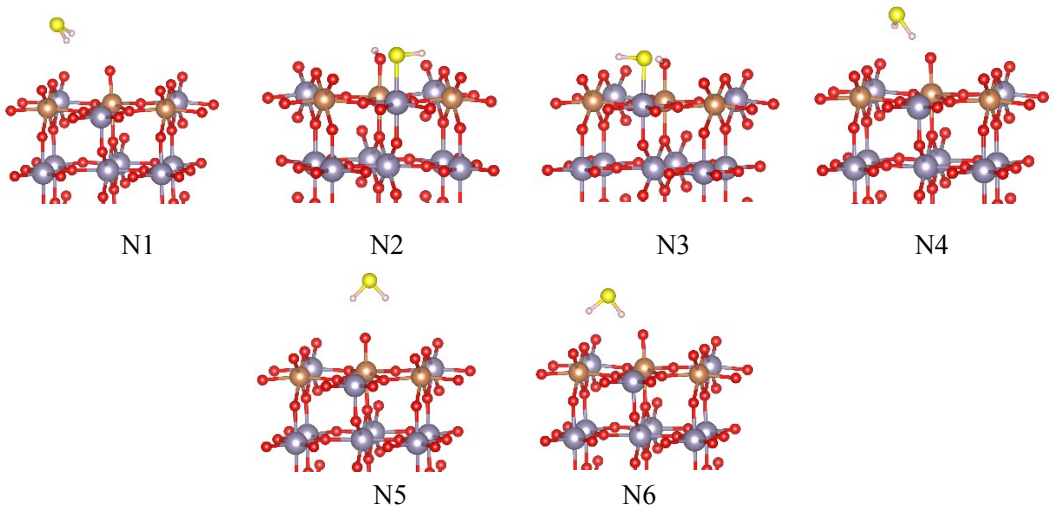


Fig. S8 Optimized structure of H_2S at different positions on the surface of $Sb_{5c6c}/SnO_2(110)$ with preadsorbed O^-. (N1-N6) H_2S molecular is adsorbed respectively at the sites of O_b; O_p; Sn_{5c}; Sn_{6c}; $O(Sb_{5c})$ and Sb_{6c} on the surface. $O(Sb_{5c})$ represents O adsorbed on Sb_{5c}.