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

The first-principles study of nH-V_{Sn}complex impurities effects in p-type SnO monolayer

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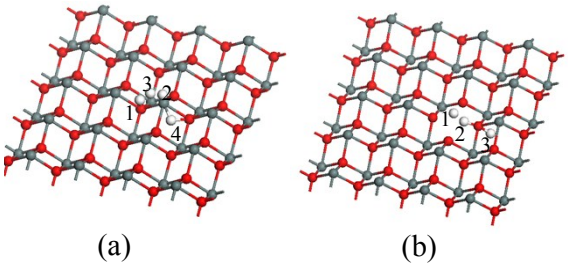

(a) (b)

Fig. S1 (a) four initial positions for H atom in H_i, (b) three initial positions for H atom in H-V_{Sn}.

Table. S1 The total energies in different charge states for four H_i initial positions in Fig. S1(a) and three H-V_{Sn} initial positions in Fig. S1(b) after relax.

	total energy(eV) for H_i				total energy(eV) for H-V_{Sn}		
	1	2	3	4	1	2	3
0	-364.8996	-364.9157	-364.1463	-365.1927	-358.4531	-361.3345	-360.7871
-1	-365.9629	-367.1982	-366.5177	-366.0481	-361.3043	-364.0821	-363.4637
+1	-363.7871	-363.6252	-362.2930	-363.8007	-	--	--

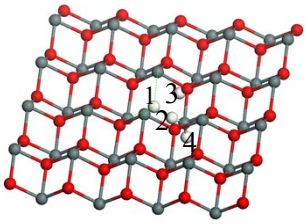

Fig. S2 Four initial positions for H atom in H-V_O.

Table. S2 The total energies for four H-V_O initial positions in Fig. S2 after relax.

position	total energy(eV)
1	-357.0911
2	-357.2232
3	-356.3364
4	-356.9181

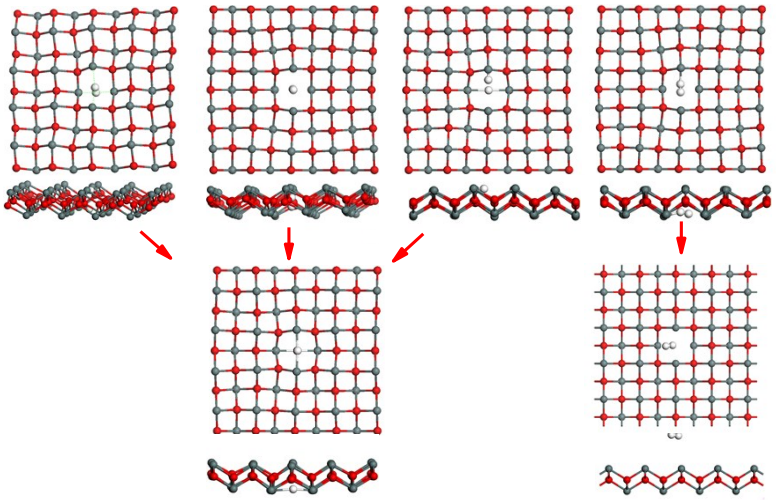

Fig .S3 The top and side view of four initial positions(top) for H atoms in 2H-V_O and their relax results(bottom) with total energies.

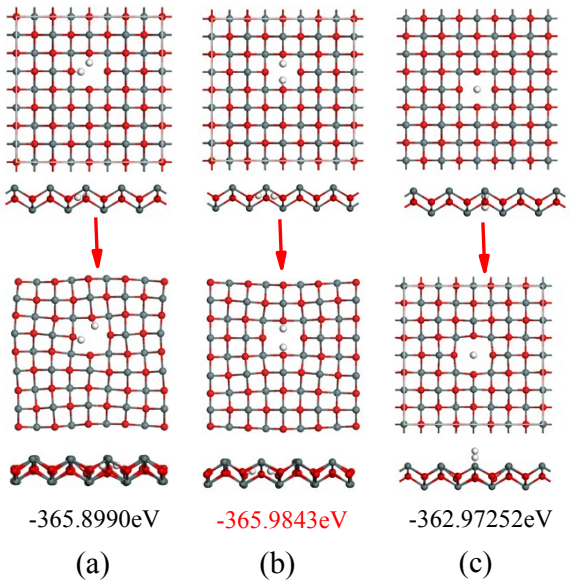

Fig. S4 The top and side view of three initial positions(top) for H atoms in 2H-V_{Sn} and their relax results(bottom) with total energies.

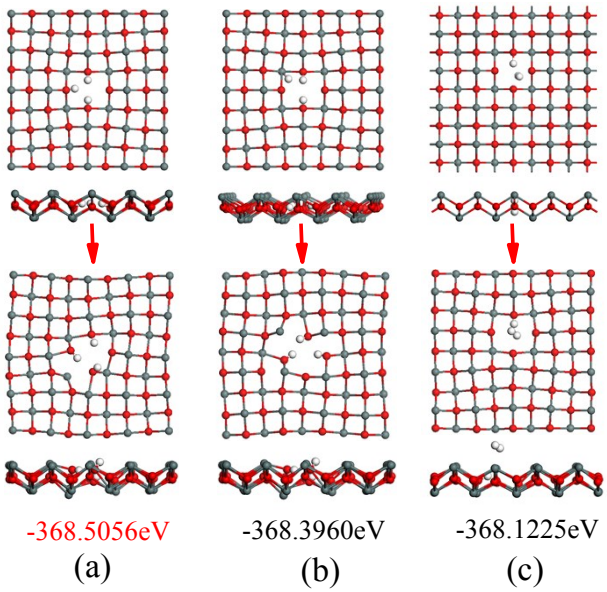

Fig. S5 The top and side view of three initial positions(top) for H atoms in 3H-V_{Sn} and their relax results(bottom) with total energies.

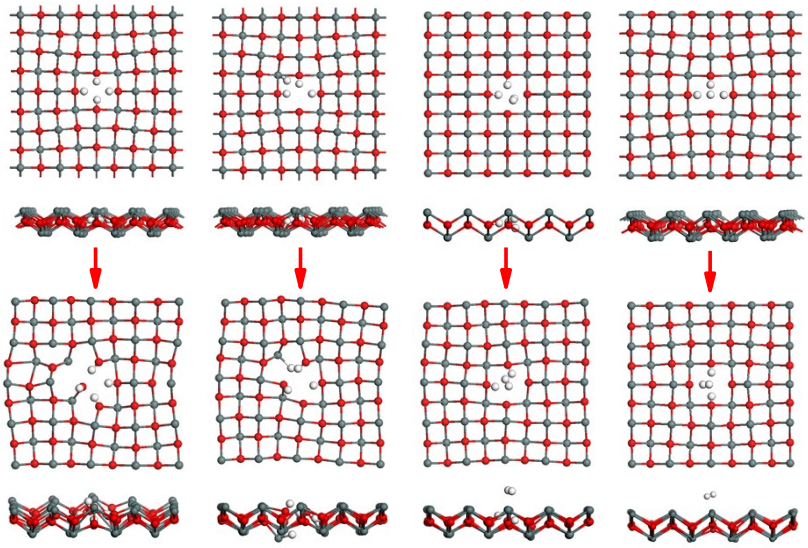

Fig. S6 The top and side view of four initial positions(top) for H atoms in 4H-V_{Sn} and their relax results(bottom) with total energies.