

Supplementary Documents

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1. System optimization and adsorption energy calculation

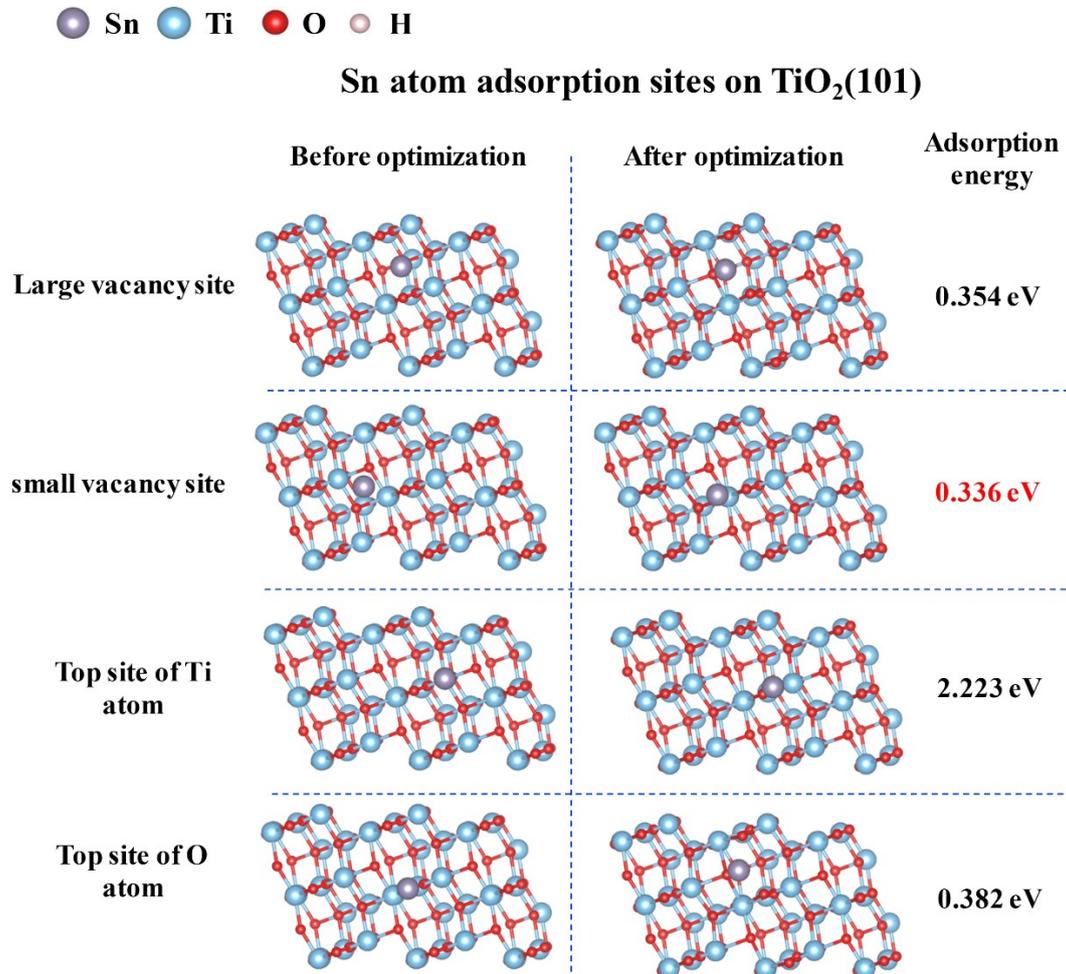


Figure 1. Adsorption sites of Sn atoms on TiO₂(101) surface and their corresponding adsorption energies.

H atom adsorption sites on TiO₂(101)

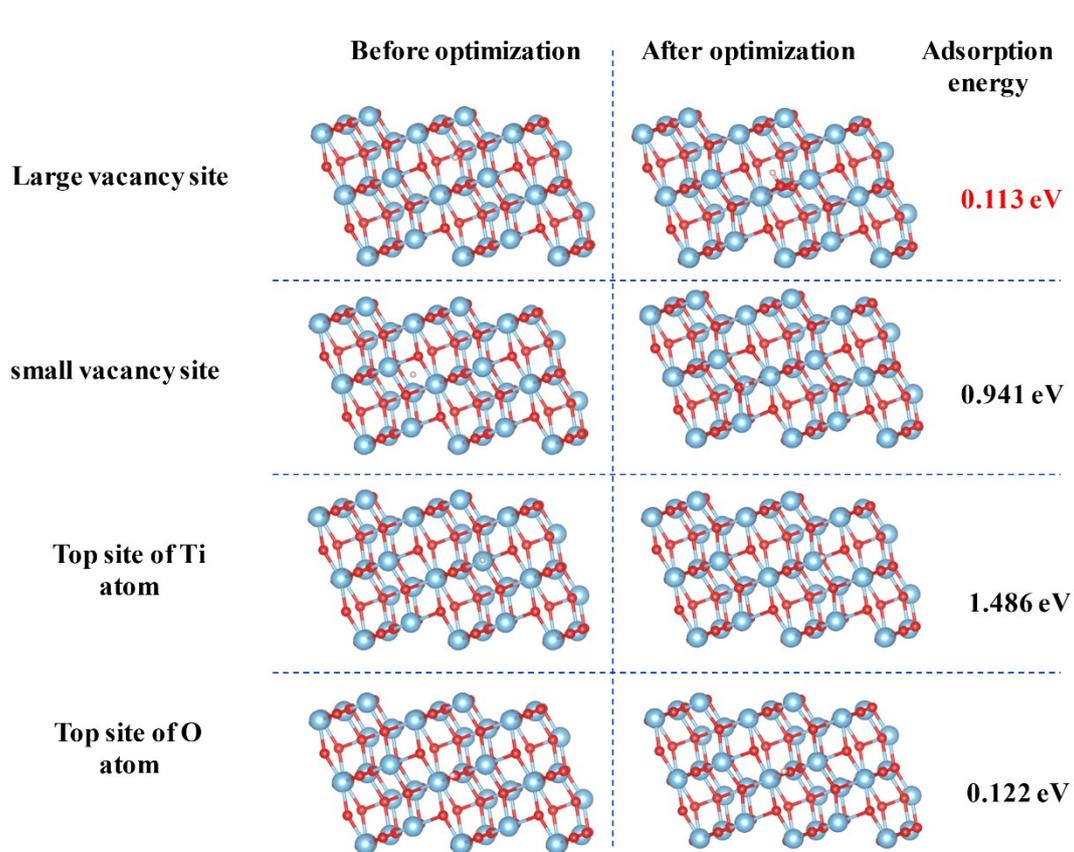


Figure 2. Adsorption sites of H atoms on TiO₂(101) surface and their corresponding adsorption energies.

Sn atom adsorption sites on TiO₂(110)

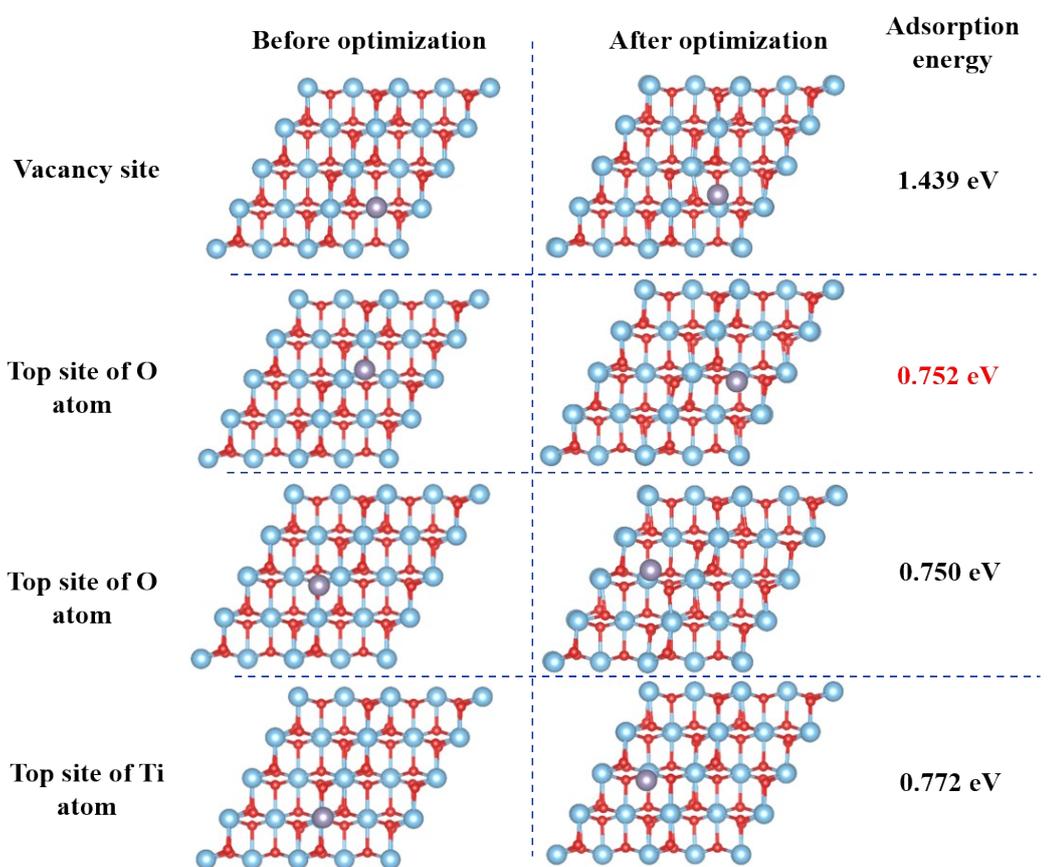


Figure 3. Adsorption sites of Sn atoms on TiO₂(110) surface and their corresponding adsorption energies.

H atom adsorption sites on TiO₂(110)

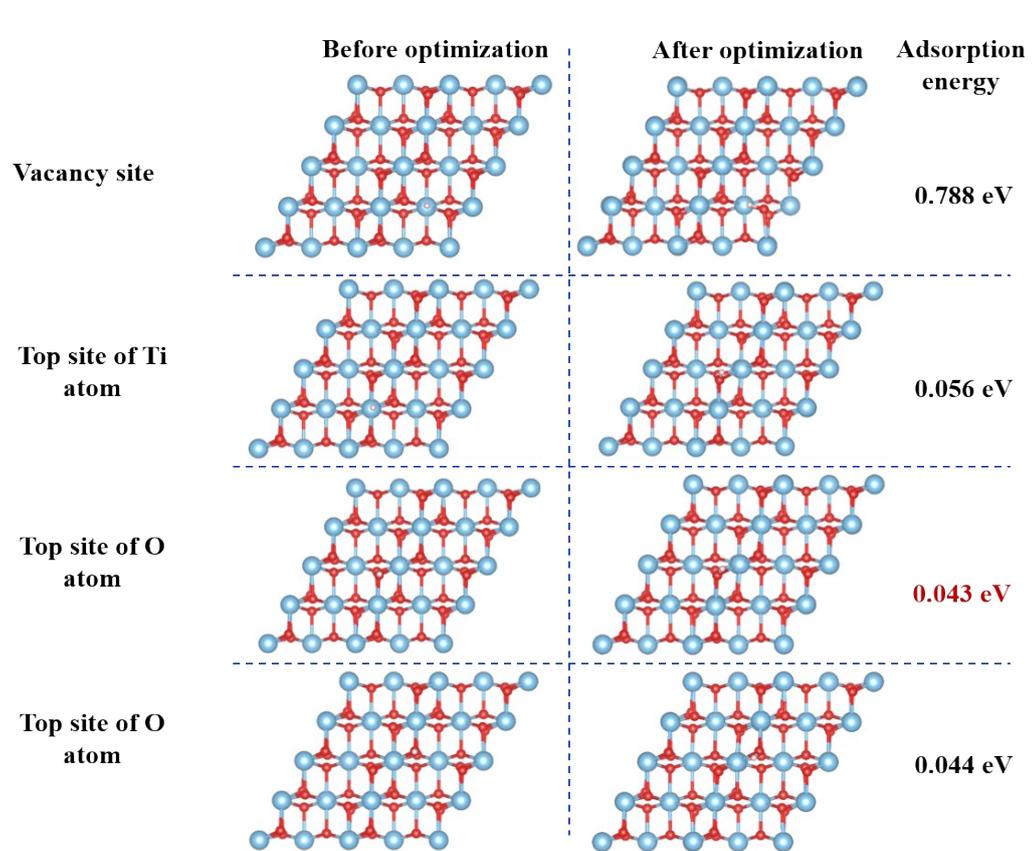
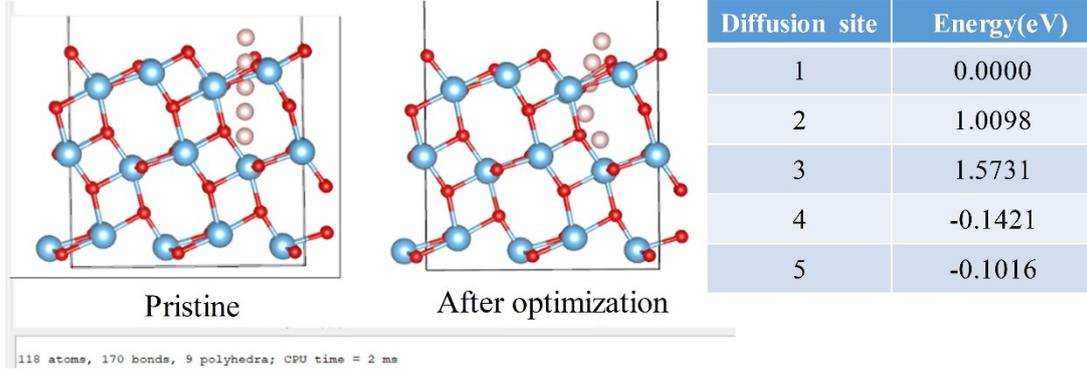


Figure 4. Adsorption sites of H atoms on TiO₂(110) surface and their corresponding adsorption energies.

2. Diffusion of H in TiO₂

Diffusion Path

(a) From the surface to the first layer



(b) From the first layer to the second layer

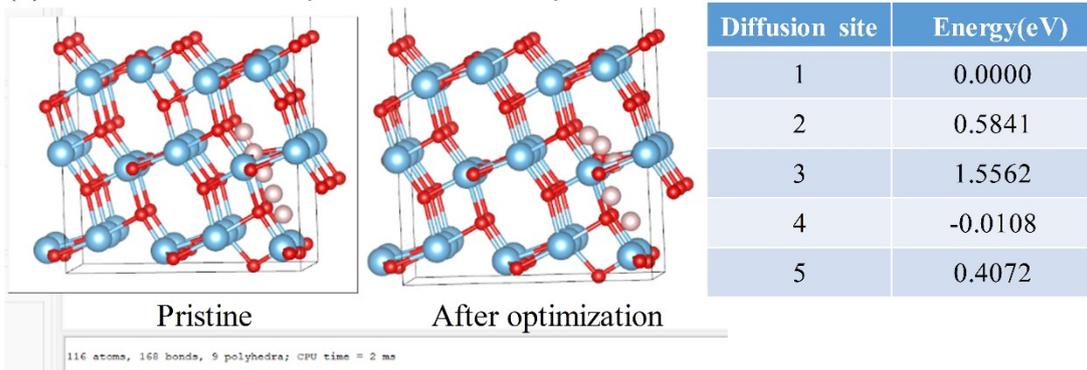
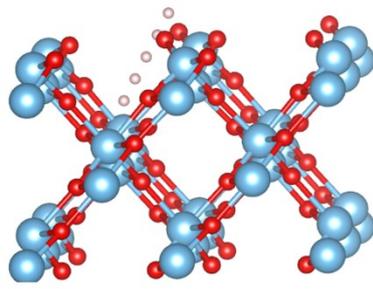


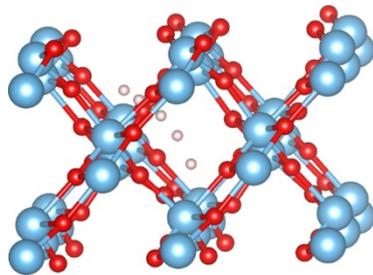
Figure 5. Diffusion pathways and transition state energies of H in TiO₂(101).

From the surface to the first layer



Diffusion site	Energy(eV)
1	0
2	0.9298
3	1.9606
4	2.4152
5	0.2372

From the first layer to the second layer



Diffusion site	Energy(eV)
1	0
2	0.2552
3	0.51
4	0.0796
5	0.2377

Figure 6. Diffusion pathways and transition state energies of H in TiO₂(110).

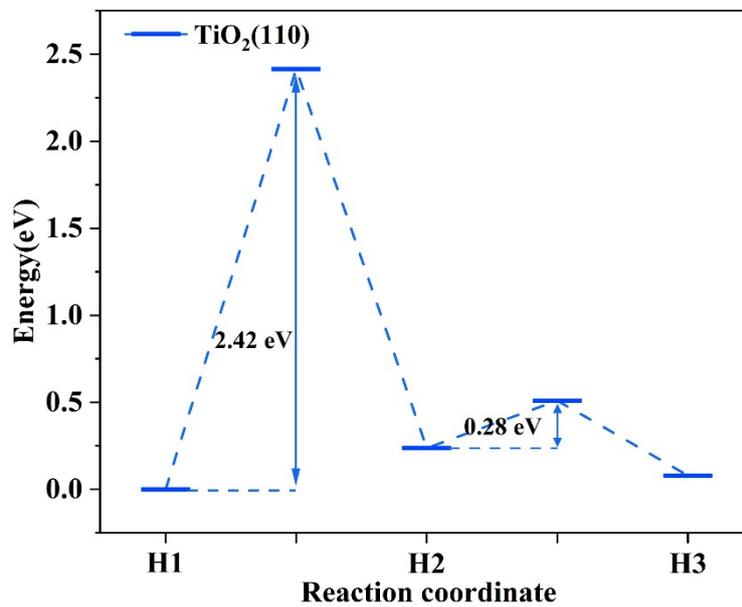


Figure 7. Diffusion of H atoms from TiO₂(110) surface to the second layer.

3. Morphology characterization by AFM

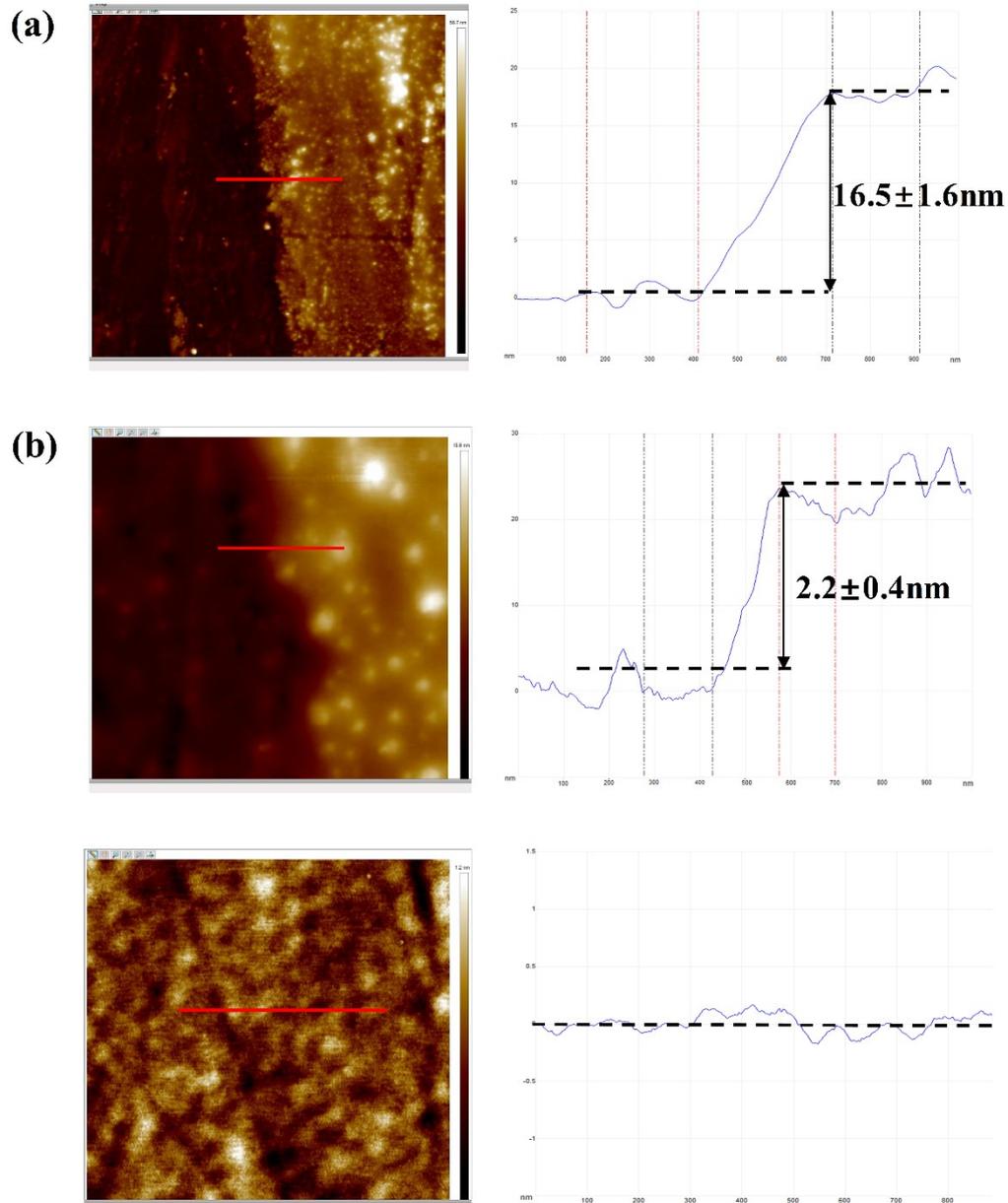


Figure 8. Step diagram of Sn contamination on TiO₂ surface after cleaning for 3 hours (a), 6 hours (b), and 9 hours.

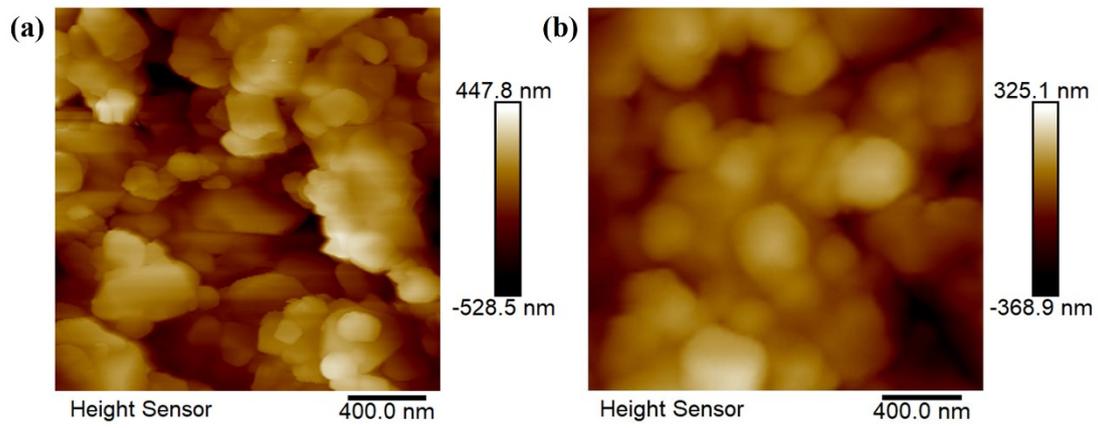


Figure 9. Morphological evolution of RuO₂ surface (a) original sample (b) after hydrogen plasma irradiation for 24 h.