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

Supplementary Information

Adsorption and sensing performance of air pollutants on β-TeO_2 monolayer: A first-principles study

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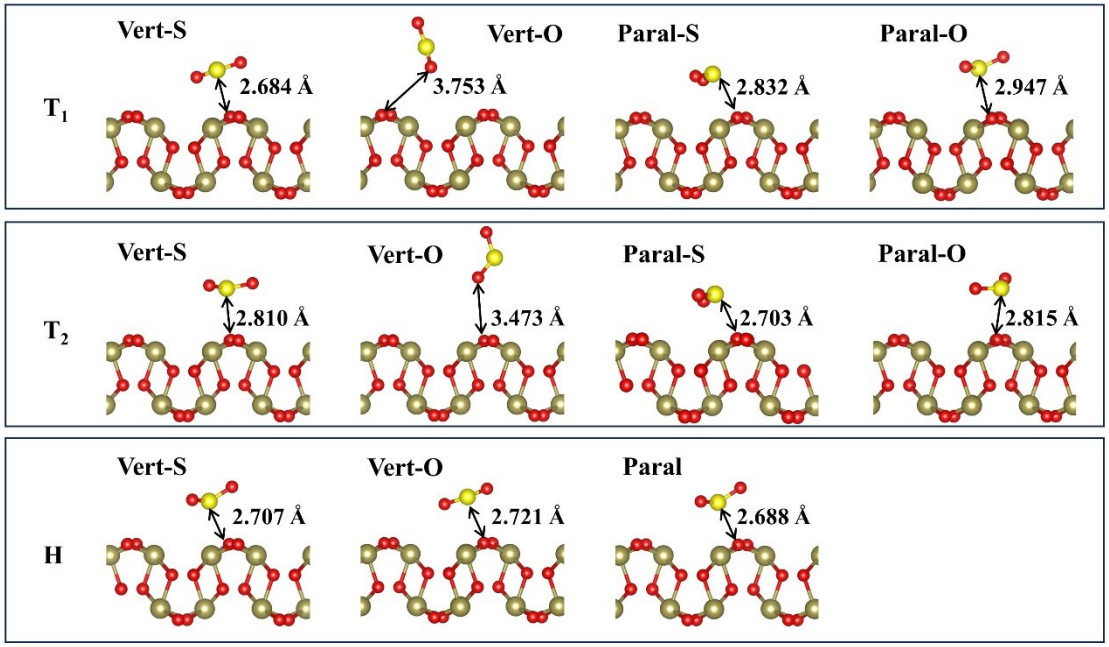

Fig. S1 The optimized atomic structures for SO_2 adsorbed on β-TeO_2 monolayer by different sites and different orientations.

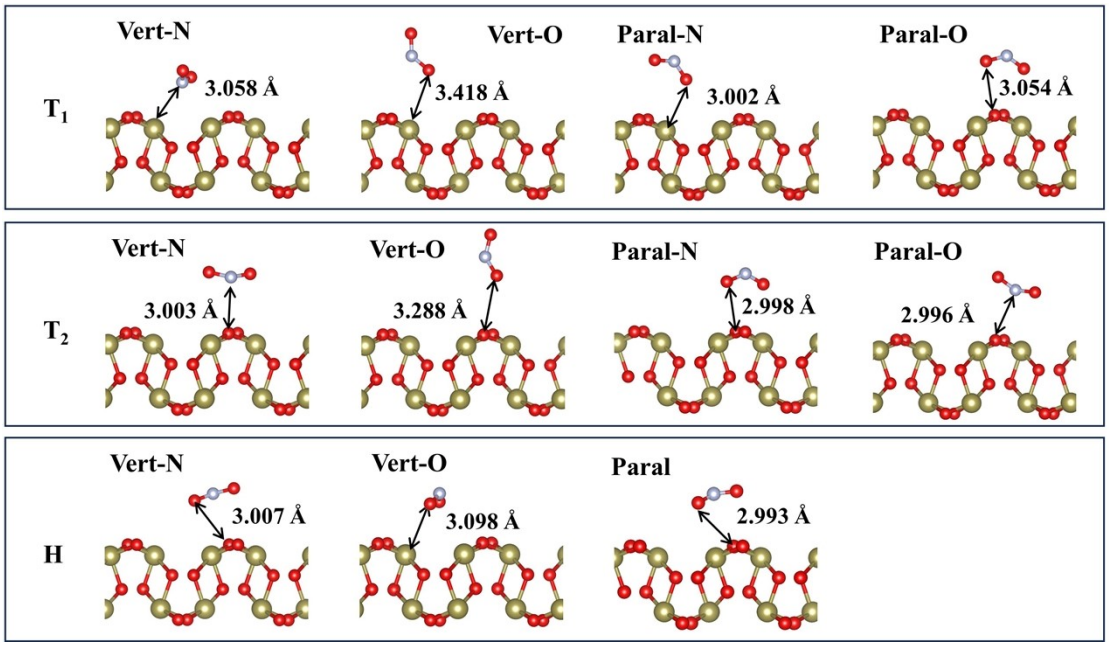

Fig. S2 The optimized atomic structures for NO_2 adsorbed on β-TeO_2 monolayer by different sites and different orientations.

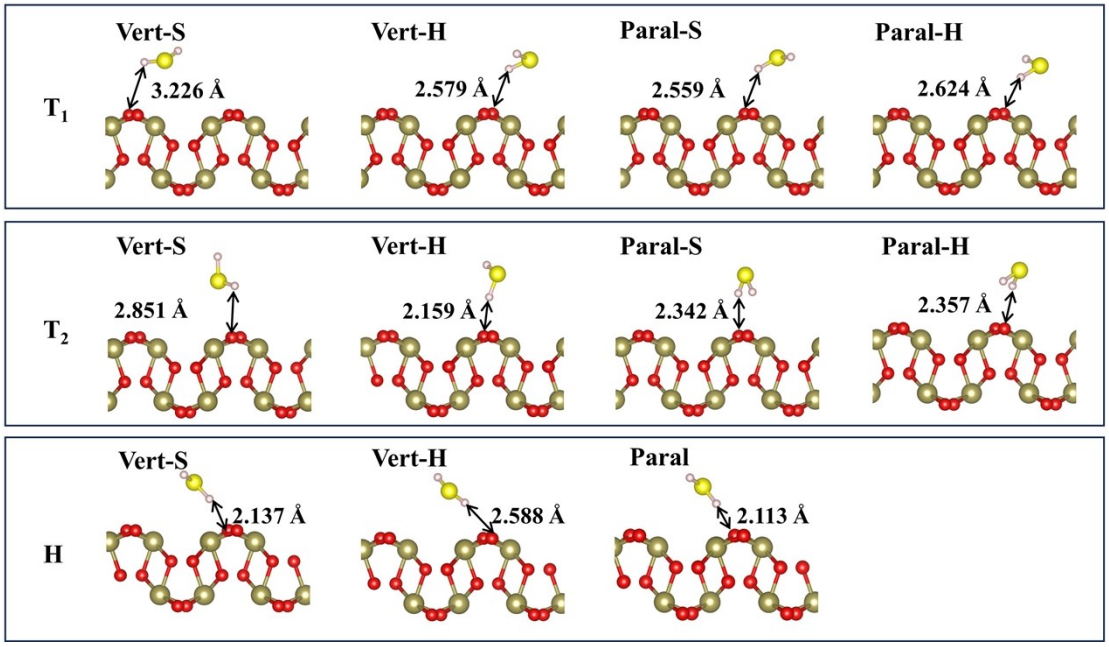

Fig. S3 The optimized atomic structures for H_2S adsorbed on β-TeO_2 monolayer by different sites and different orientations.

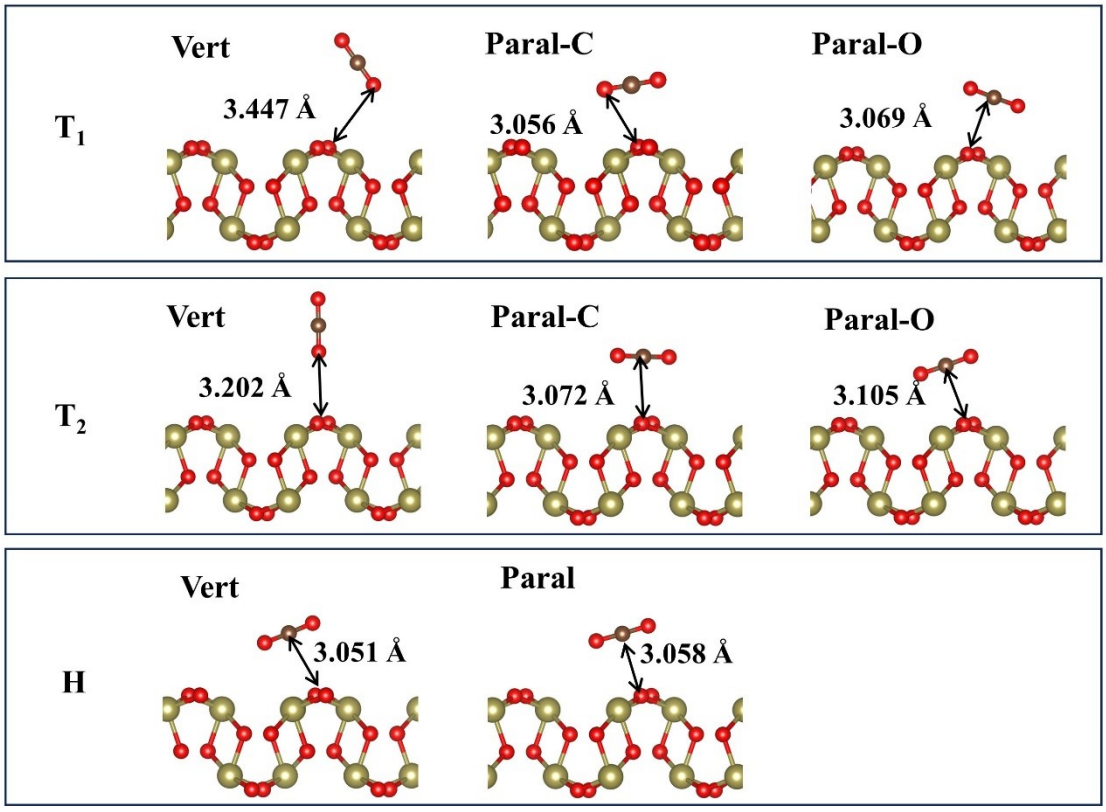

Fig. S4 The optimized atomic structures for CO_2 adsorbed on β-TeO_2 monolayer by different sites and different orientations.

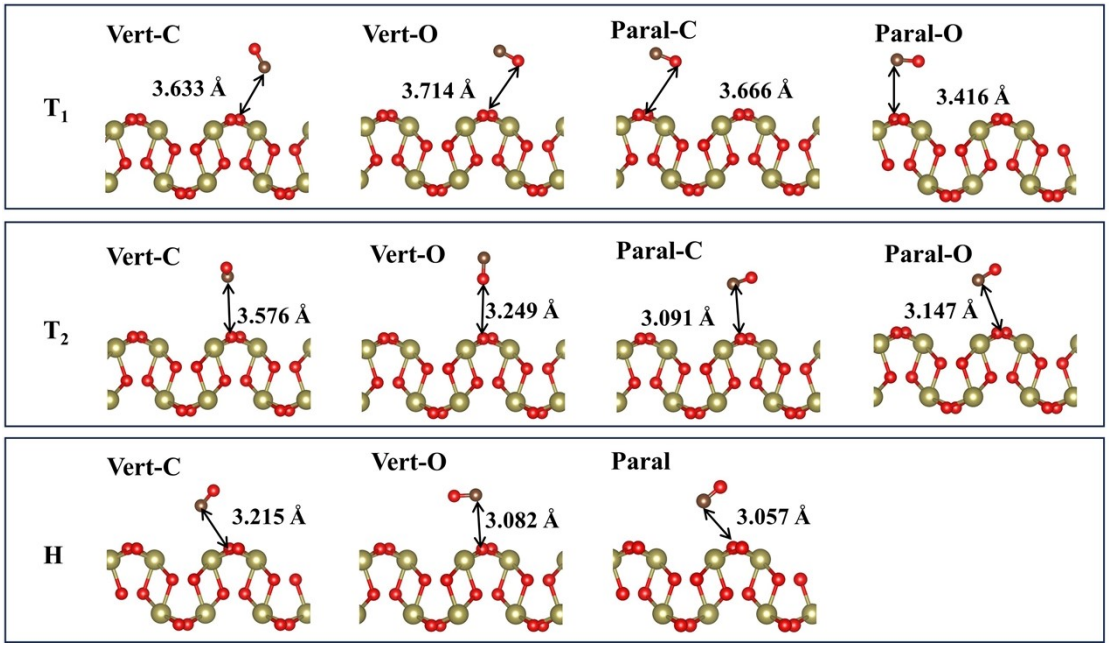

Fig. S5 The optimized atomic structures for CO adsorbed on β-TeO_2 monolayer by different sites and different orientations.

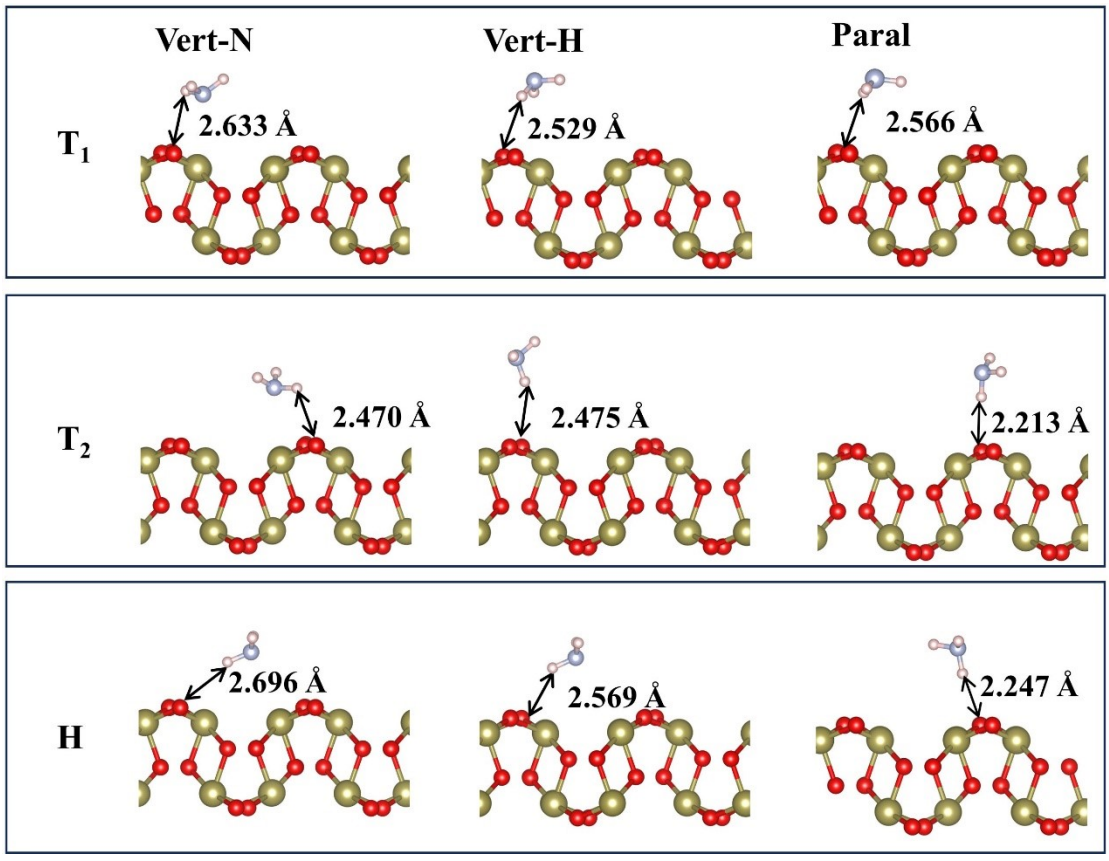

Fig. S6 The optimized atomic structures for NH_3 adsorbed on β-TeO_2 monolayer by different sites and different orientations.

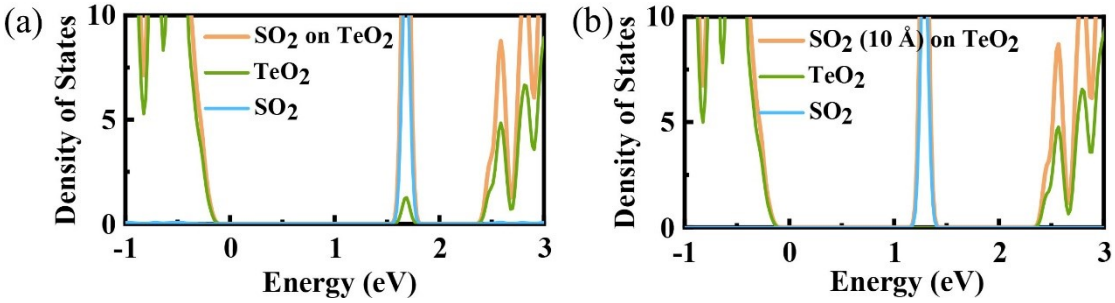

Fig. S7 The PDOS of (a) SO_2 adsorbed on the β-TeO_2 monolayer and (b) the system where SO_2 is positioned 10 Å above the β-TeO_2 monolayer. The Fermi level is assigned to 0 eV.

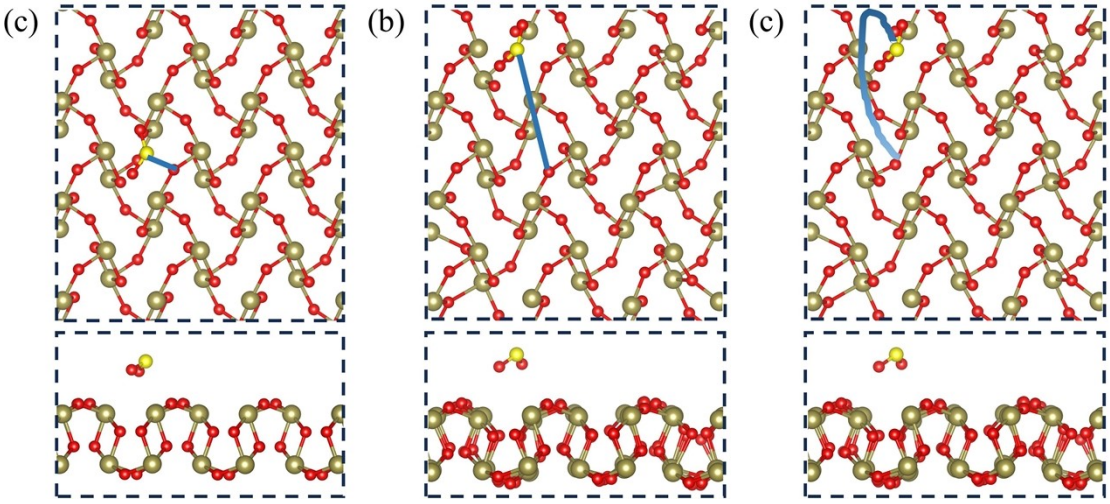

Fig. S8 Results of AIMD simulations performed for SO_2 on β-TeO_2 monolayer: the atomic structures at (a) 0 ps and (b) 5 ps, and (c) projection of gas molecule trajectory.

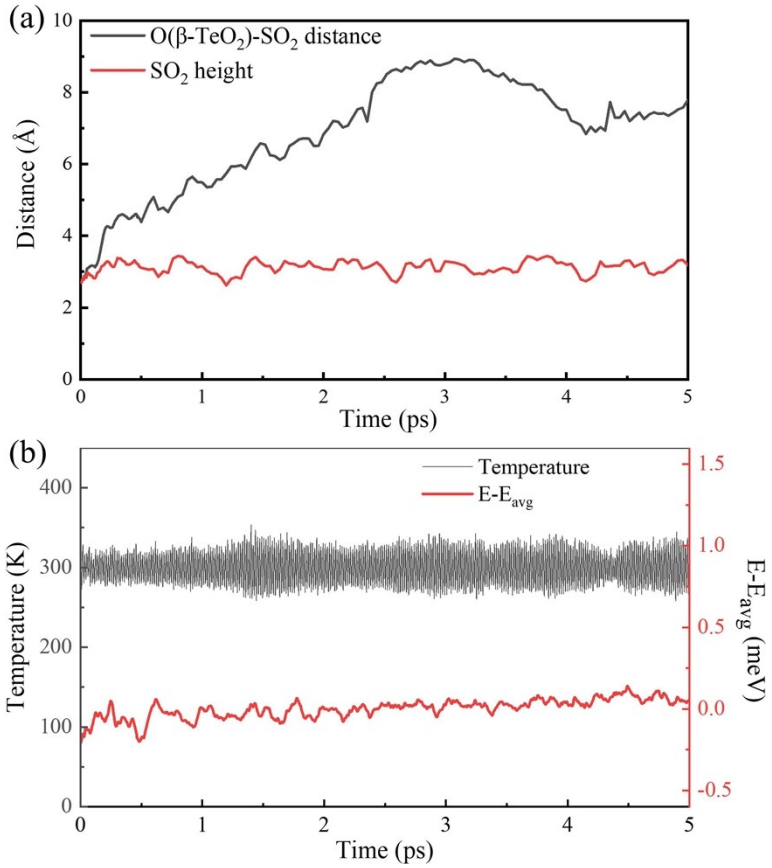

Fig. S9 Results of AIMD simulations performed for SO_2 adsorbed on β-TeO_2 monolayer at 300 K: (a) time dependencies of O(β-TeO_2)-SO_2 distance and SO_2 height above β-TeO_2 monolayer, (b) variation of total energy during simulations.

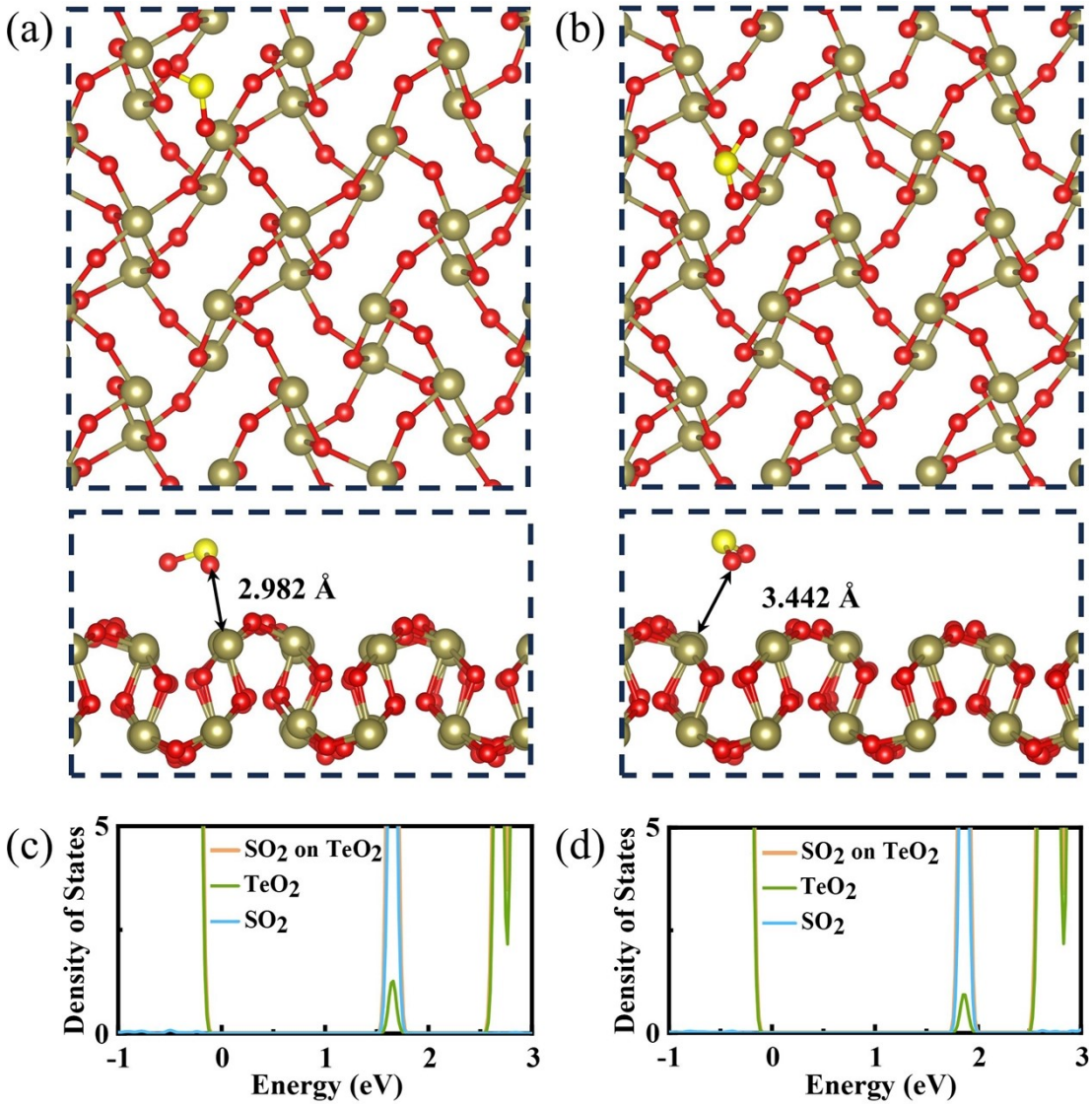

Fig. S10 Atomic structures and the related projected density of states of two alternative adsorption configurations with the adsorption distances of 2.982 Å and 3.442 Å during the AIMD simulations.