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# Supplementary Information for: Computational investigation of gas detection and selectivity on $TiS_3$ nanoflakes supported by experimental evidence

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## List of Figures



**Note: In all figures S7 to S16, only the slab atoms of configuration No.1 are visible, that is, all Ti and S atoms that belong to the other configurations are hidden for clarity.**

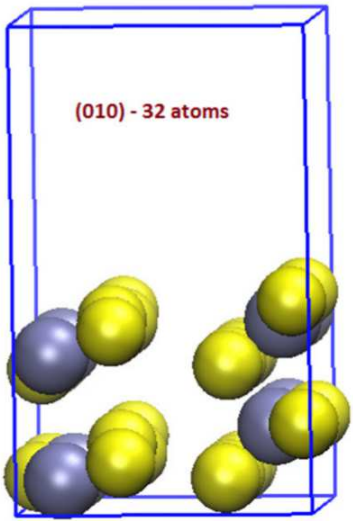


**Fig. S1** Computational slab model for surface (010) having 32 atoms.

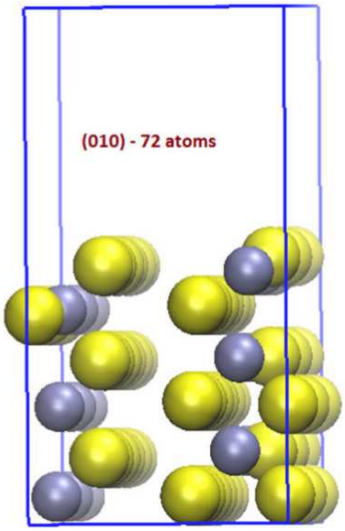


**Fig. S2** Computational slab model for surface (010) having 72 atoms.

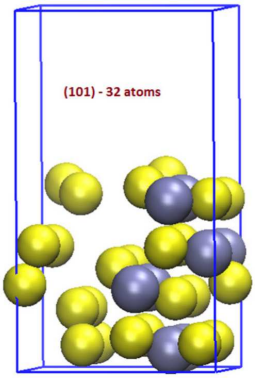


**Fig. S3** Computational slab model for surface (101) having 32 atoms.

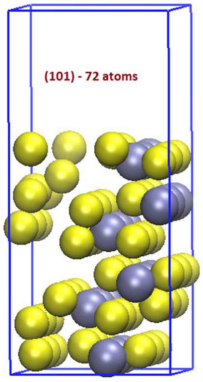


**Fig. S4** Computational slab model for surface (101) having 72 atoms.

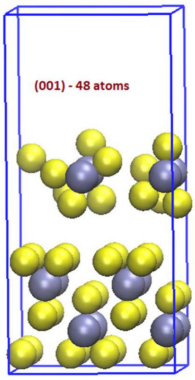


**Fig. S5** Computational slab model for surface (001) having 48 atoms.

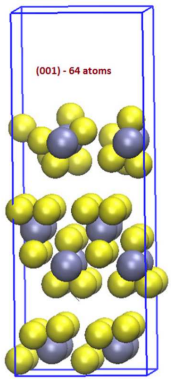


**Fig. S6** Computational slab model for surface (001) having 64 atoms.

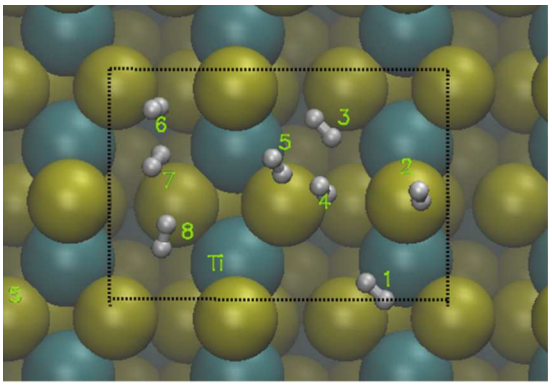


**Fig. S9** Optimized structure of adsorbed $H_2$ molecule on defect free (001). Each number corresponds to a separate calculation.

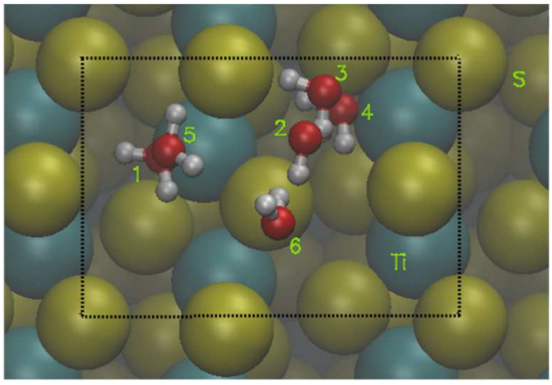


**Fig. S7** Optimized structure of adsorbed $H_2O$ molecule on defect free (001). Each number corresponds to a separate calculation. Only one slab surface is visible.

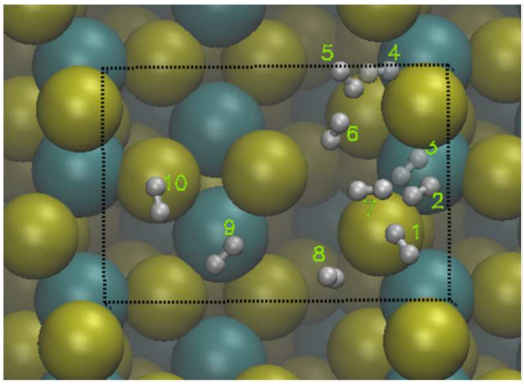


**Fig. S10** Optimized structure of adsorbed $H_2$ molecule on double S-deficient (001). Each number corresponds to a separate calculation.

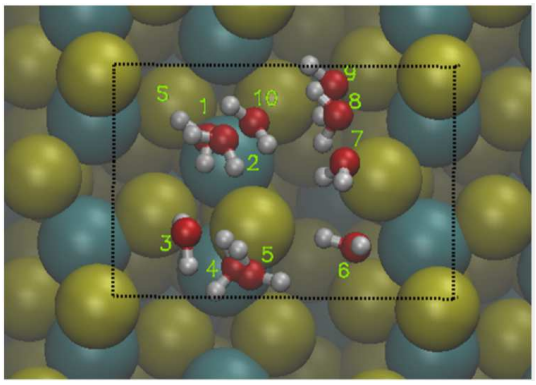


**Fig. S8** Optimized structure of adsorbed $H_2O$ molecule on double S-deficient (001). Each number corresponds to a separate calculation.

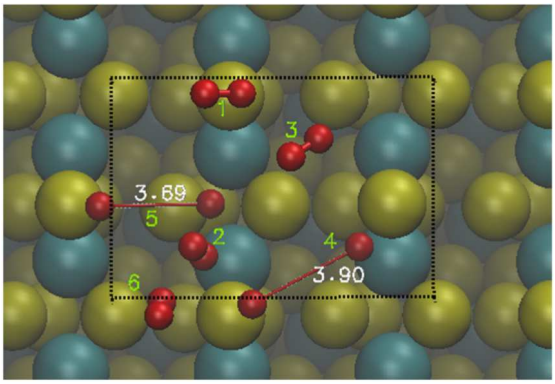


**Fig. S11** Optimized structure of adsorbed $O_2$ molecule on defect free (001). Each number corresponds to a separate calculation. Those O-O pairs falling at more than 3 Å apart indicate dissociative adsorption.

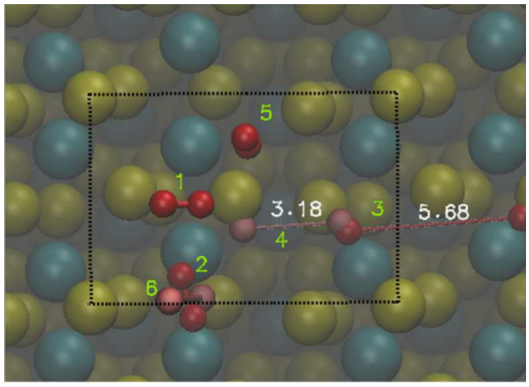


**Fig. S12** Optimized structure of adsorbed $O_2$ molecule on double S-deficient (001). Each number corresponds to a separate calculation. Those O-O pairs falling at more than 3 Å apart indicate dissociative adsorption.

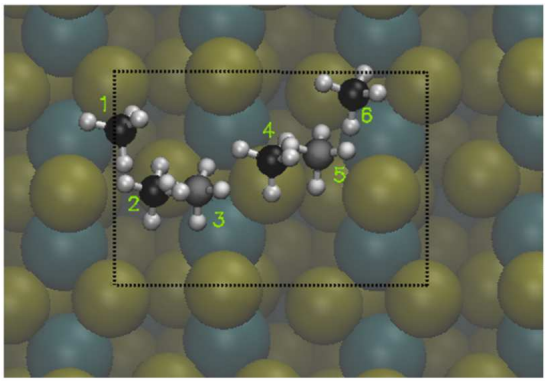


**Fig. S13** Optimized structure of adsorbed $CH_4$ molecule on defect free (001). Each number corresponds to a separate calculation.

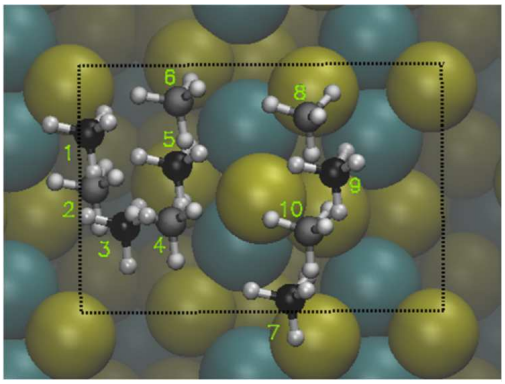


**Fig. S14** Optimized structure of adsorbed $CH_4$ molecule on double S-deficient (001). Each number corresponds to a separate calculation.

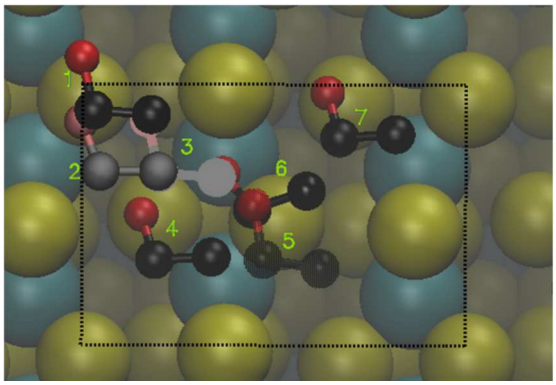


**Fig. S15** Optimized structure of adsorbed $C_2H_5OH$ molecule on defect free (001). Each number corresponds to a separate calculation.

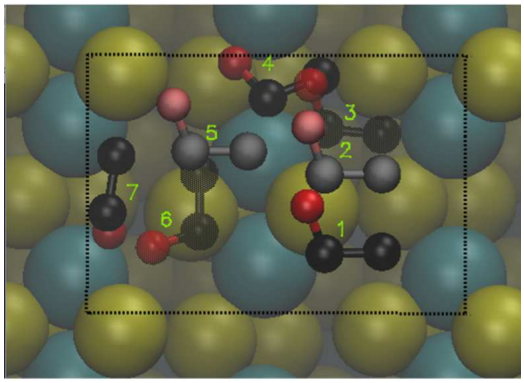


**Fig. S16** Optimized structure of adsorbed $C_2H_5OH$ molecule on double S-deficient (001). Each number corresponds to a separate calculation.

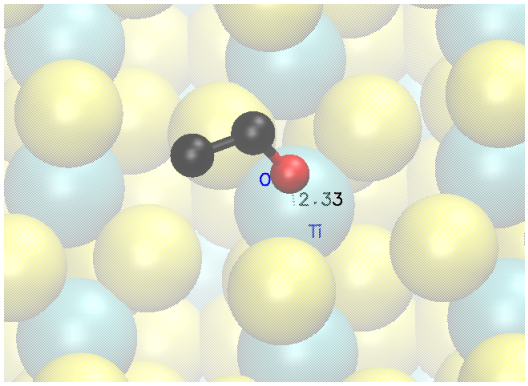


**Fig. S17** Geometry of the ethanol molecule on the stoichiometric surface. This particular structure corresponds to the energy peak at about -1.1 eV.

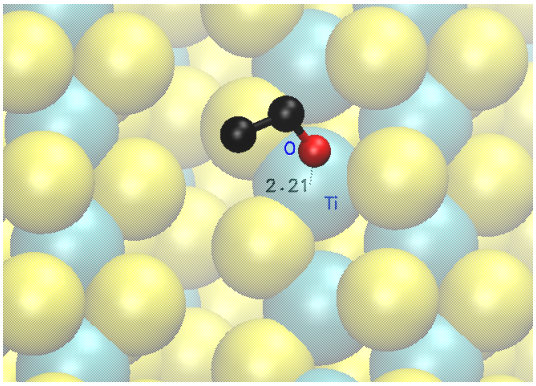


**Fig. S18** Geometry of the ethanol molecule on the double S-deficient surface. This particular structure corresponds to the energy peak at about -1.1 eV.