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## Supplementary Information for: Computational investigation of gas detection and selectivity on TiS<sub>3</sub> nanoflakes supported by experimental evidence

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

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



Fig. S2 Computational slab model for surface (010) having 72 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. S15 Optimized structure of adsorbed  $C_2H_5OH$  molecule on defect free (001). Each number corresponds to a separate calculation.



**Fig. S13** Optimized structure of adsorbed  $CH_4$  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. S14** Optimized structure of adsorbed  $CH_4$  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.