Supporting Information

Coverage-sensitive mechanism of electrochemical NO reduction on $SrTiO_3$(001) surface: A DFT investigation

Xiangyu Zhang, [a] *Lu Liu,* [a] *Yuncai Zhao,* [a] *Yijing Gao,* *[a,b] *Deli Chen, and Weidong Zhu* *[a, b]

a. Key Laboratory of the Ministry of Education for Advanced Catalysis Materials, Institute of Physical Chemistry, Zhejiang Normal University, 321004 Jinhua, P. R. of China

b. Zhejiang Engineering Laboratory for Green Syntheses and Applications of Fluorine-Containing Specialty Chemicals, Institute of Advanced Fluorine-Containing Materials, Zhejiang Normal University, 321004 Jinhua, P. R. of China

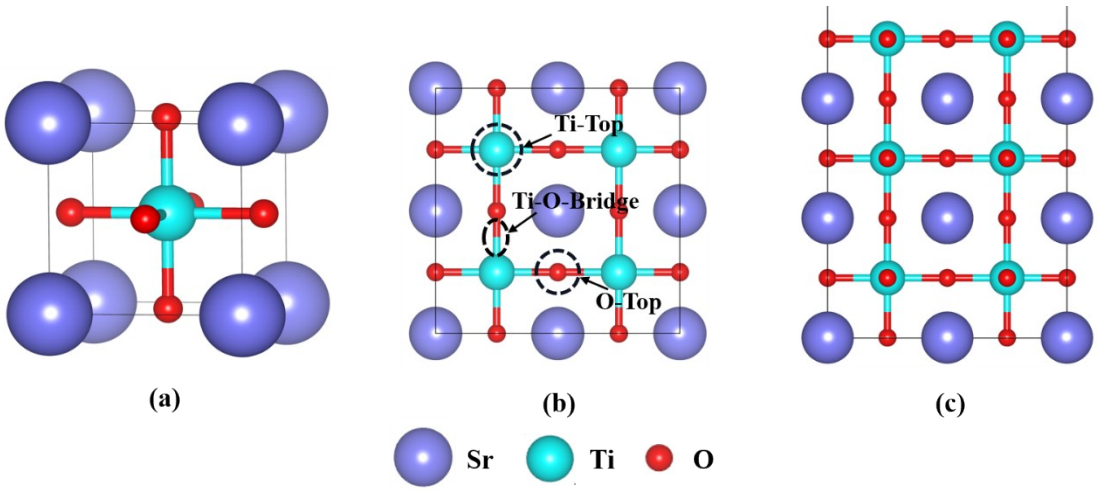

Fig. S1 Primitive cell of the chalcogenide $SrTiO_3$ (a). Top (b) and side view (c) of $SrTiO_3$ (001) surface.

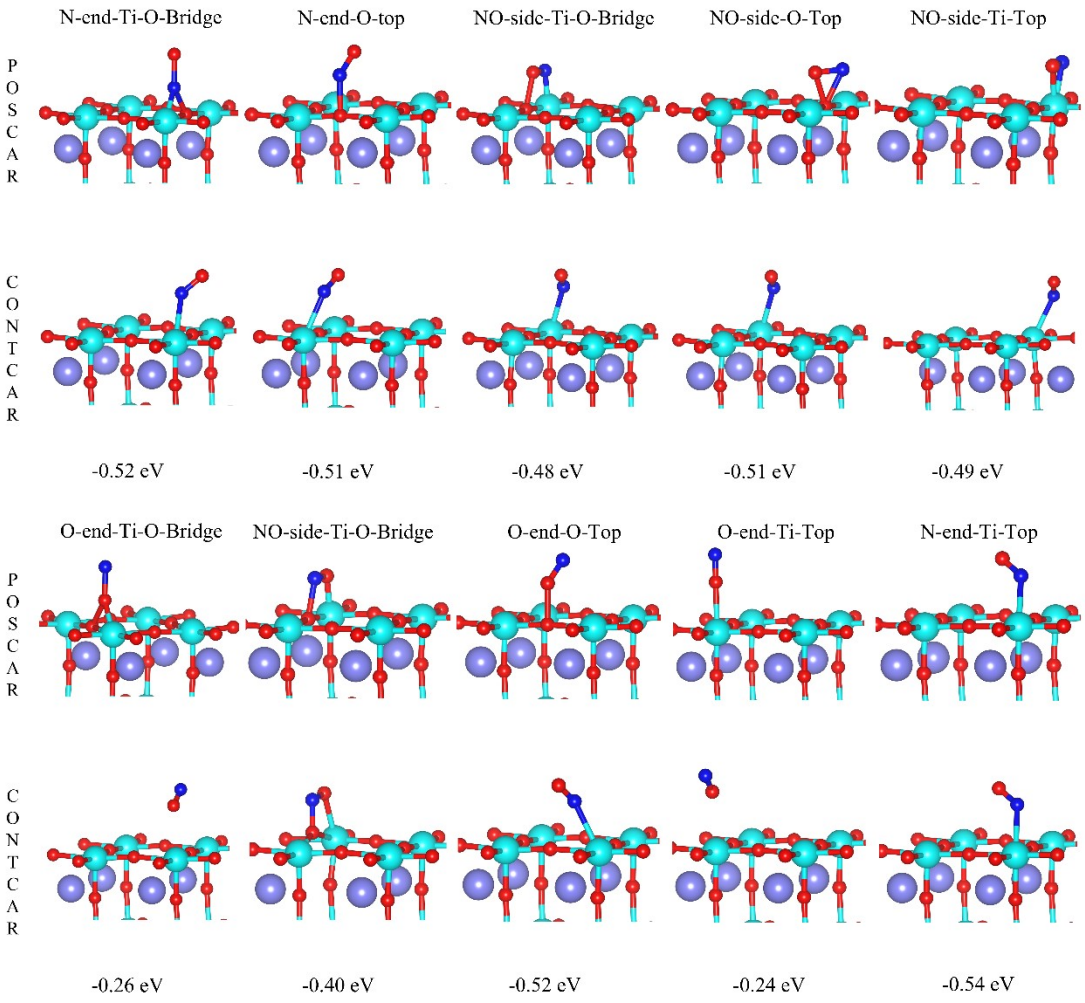

Fig. S2 NO adsorption structures and corresponding energies on $SrTiO_3$(001) at 0.25 ML.

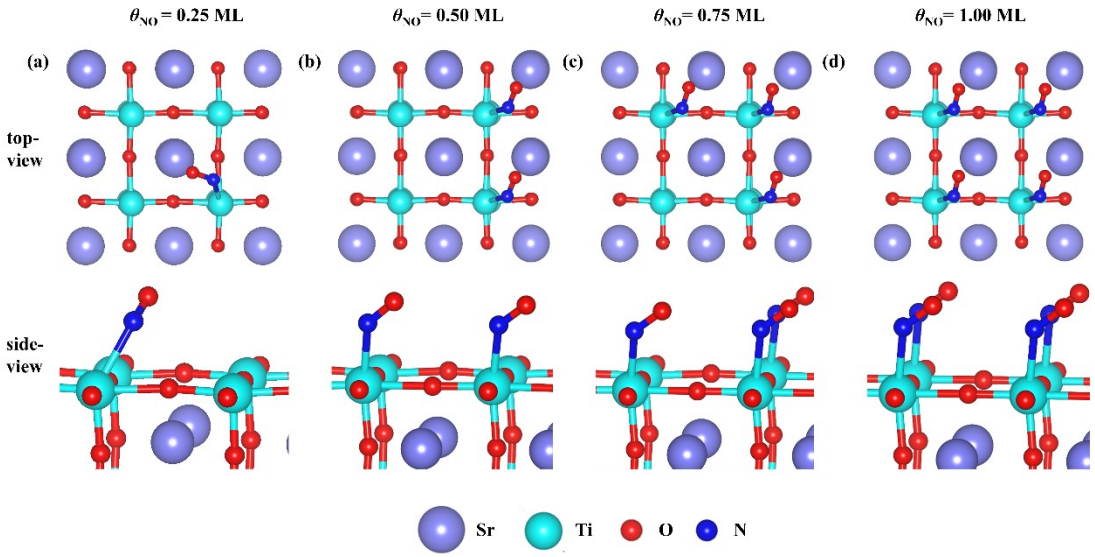

Fig. S3 Top and side views of the optimal NO adsorption structures at θ_{NO} =0.25 ML (a), 0.50 ML (b), 0.75 ML (c), and 1.00 ML (d), respectively.

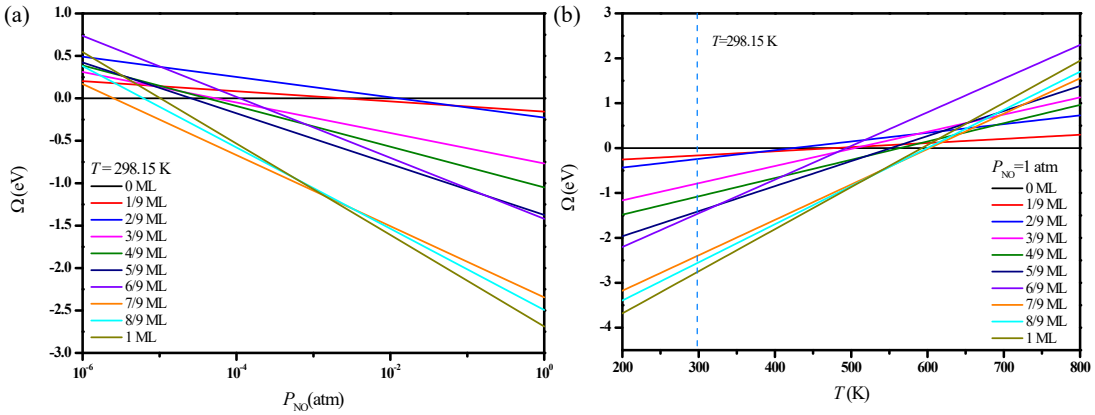

Fig. S4 Phase diagram for NO adsorption on the 3 × 3 $SrTiO_3$ (001) surface as a function of NO pressure at 298.15 K (a) and of temperature at a NO pressure of 1 atm (b).

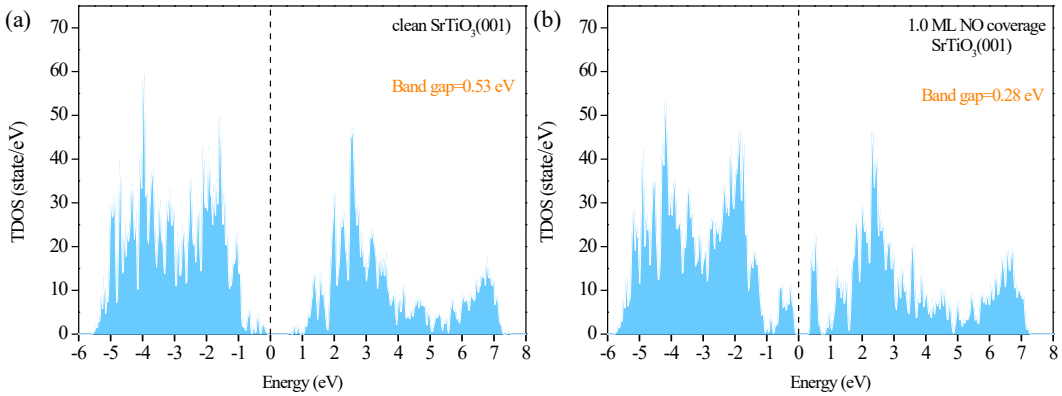

Fig. S5 Total density of states for clean $SrTiO_3$(0 0 1) surface (a) and 1.00 ML NO coverage (b), with the dashed line indicating the Fermi energy level. The corresponding band gap value is presented in each panel.

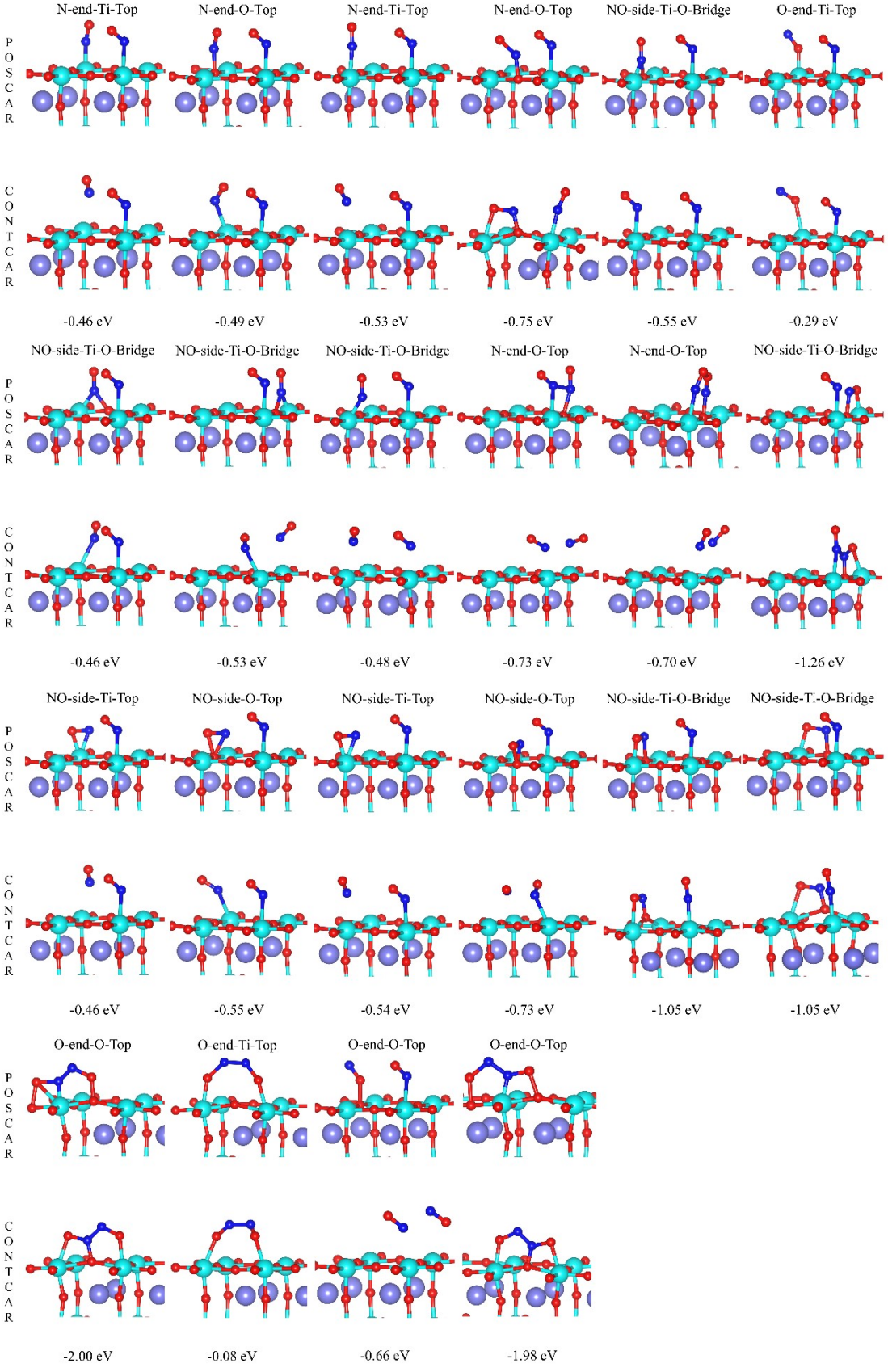

Fig. S6 NO adsorption structures and corresponding energies on $SrTiO_3$(001) at 0.50 ML.

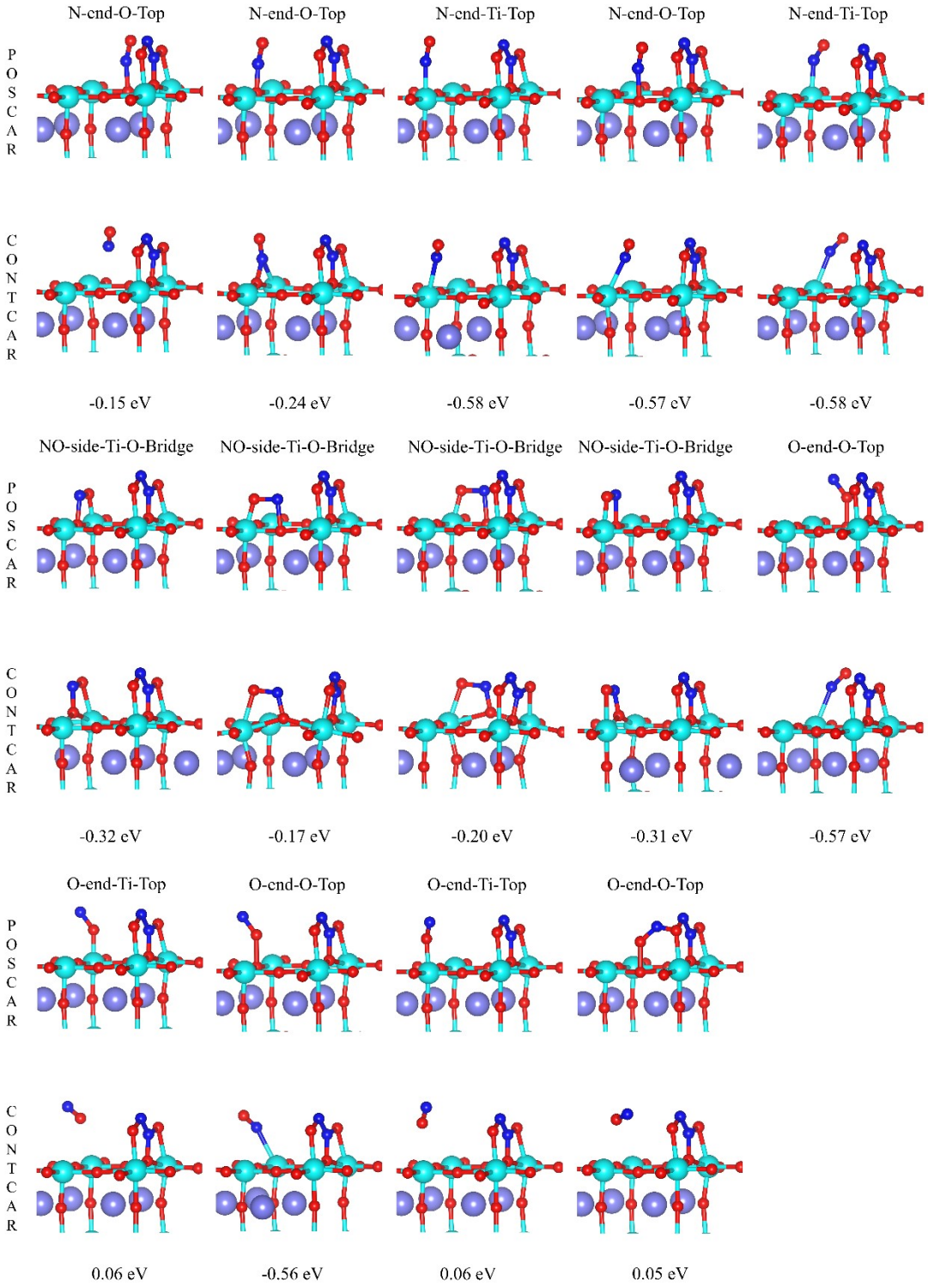

Fig. S7 NO adsorption structures and corresponding energies on $SrTiO_3$(001) at 0.75 ML.

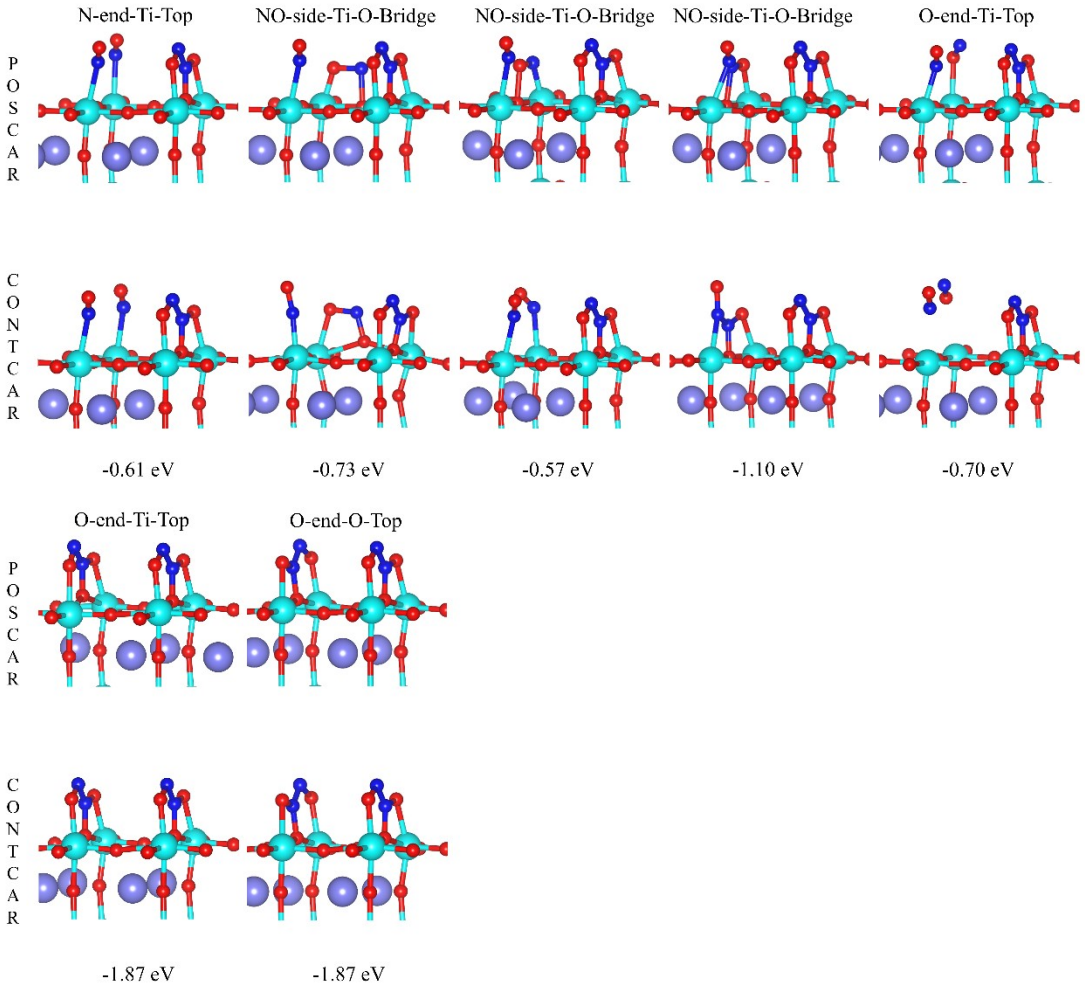

Fig. S8 NO adsorption structures and corresponding energies on $SrTiO_3$(001) at 1.00 ML.

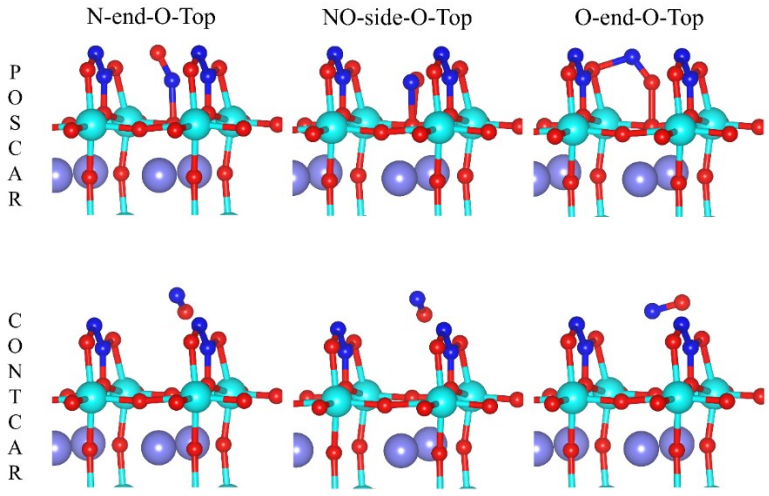

Fig. S9 Structures of five NO molecules adsorbed on $SrTiO_3$(001).

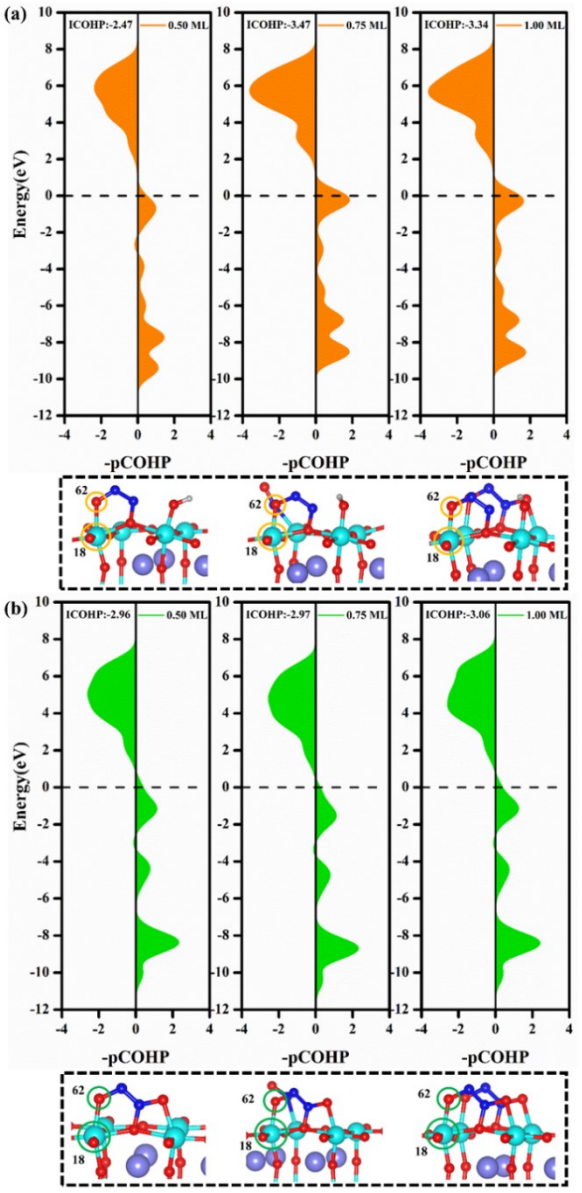

Fig. S10 COHP of the O-62 of the adsorbed intermediate *$(NO)_2$ and the active center Ti-18 (a) and of the adsorbed intermediate *ONN+*OH and the active center Ti-18 (b).

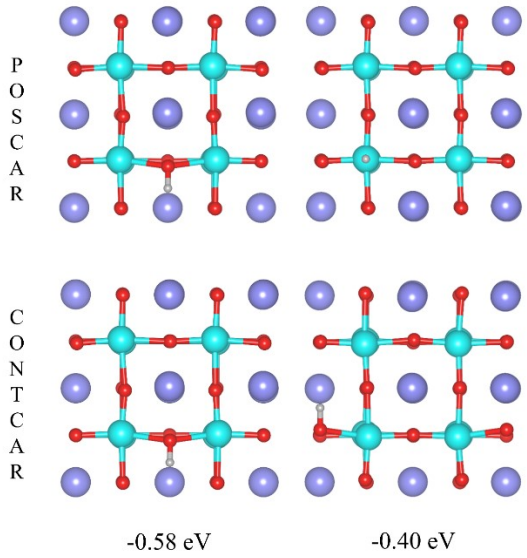

Fig. S11 Structures and corresponding energies of H adsorption on $SrTiO_3(001)$ at 0 ML.

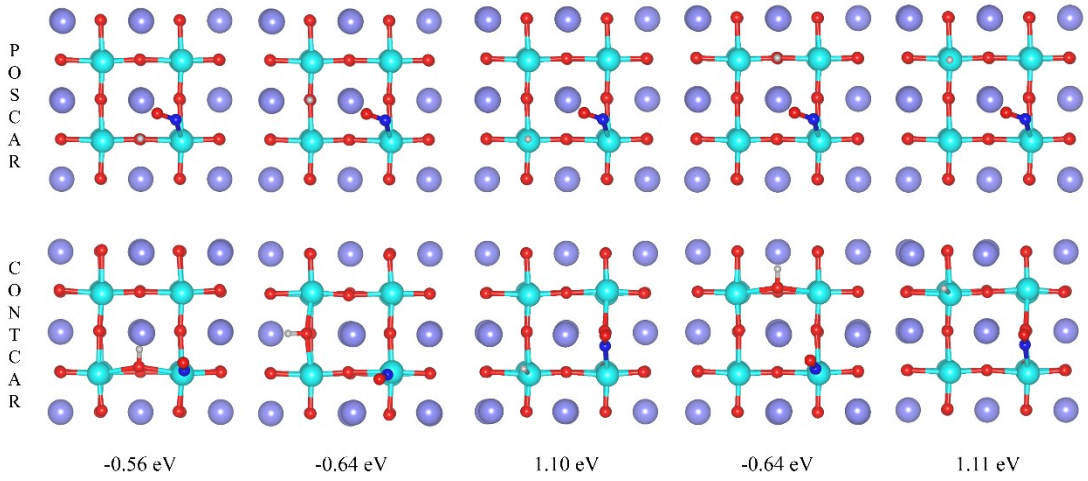

Fig. S12 Structures and corresponding energies of H adsorption on $SrTiO_3(001)$ at 0.25 ML.

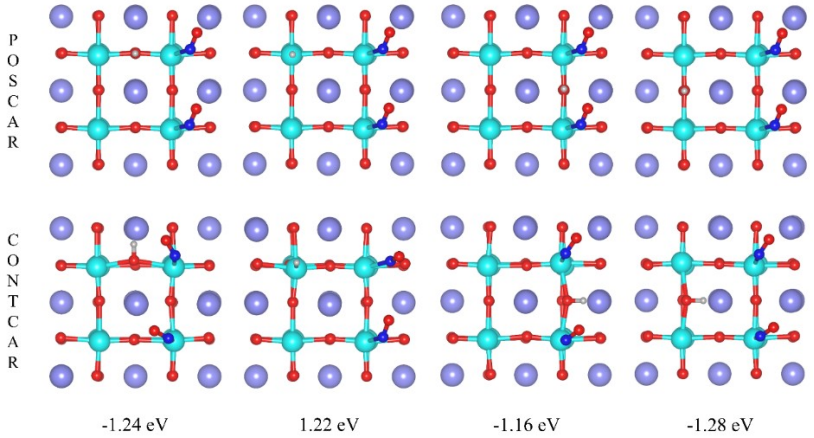

Fig. S13 Structures and corresponding energies of H adsorption on $SrTiO_3$(001) at 0.50 ML.

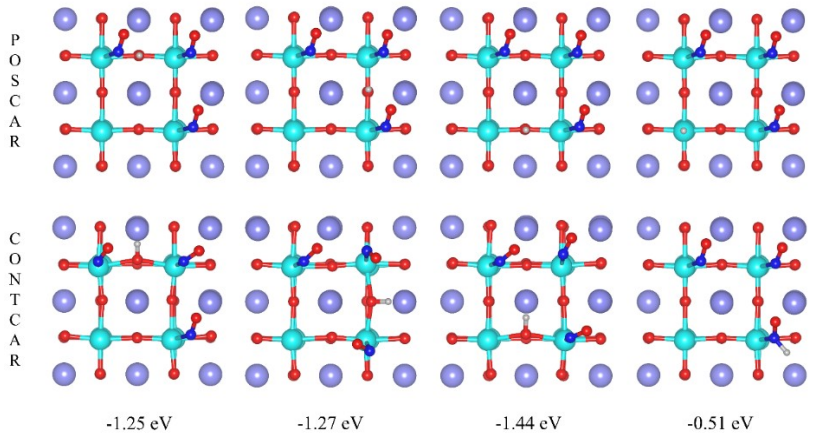

Fig. S14 Structures and corresponding energies of H adsorption on $SrTiO_3$(001) at 0.75 ML.