Supplementary Information (SI) for Catalysis Science & Technology.

Illustrating the Surface chemistry of Nitrogen Oxides (NO_x) adsorbed on Rutile TiO_2 (110) with the aid of STM and AIMD simulation.

S. Muthukrishnan[1,2], R. Vidya[1,2,] *, and Anja Olafsen Sjåstad[3]

Supplementary materials

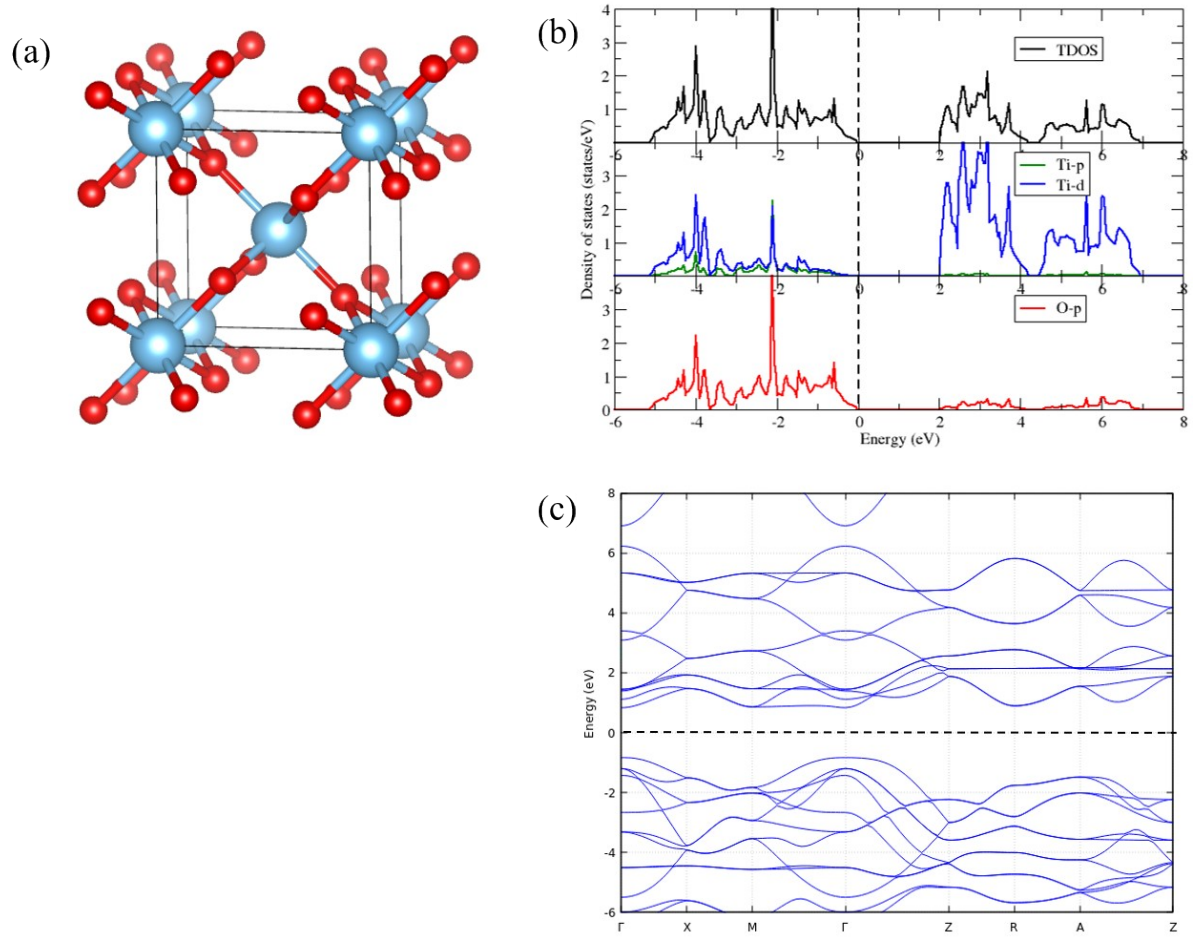

Figure S1 (a) Unit cell structure, (b) The projected density of states, and (c) electronic band structure plots for TiO_2 Rutile

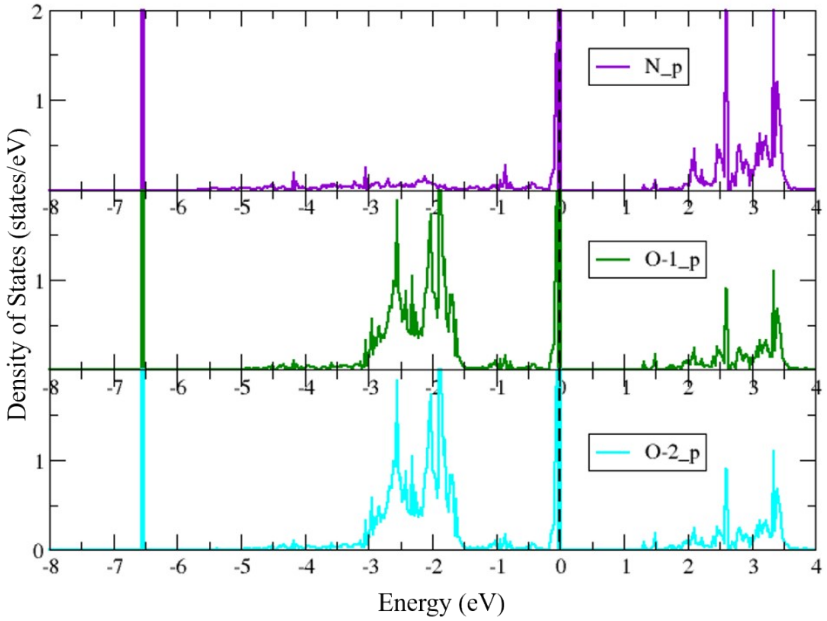

Figure S2, Projected Density of States for NO_2 molecule adsorbed on Ti_{5c} site with O down configuration on TiO_2 Rutile (110) surface.

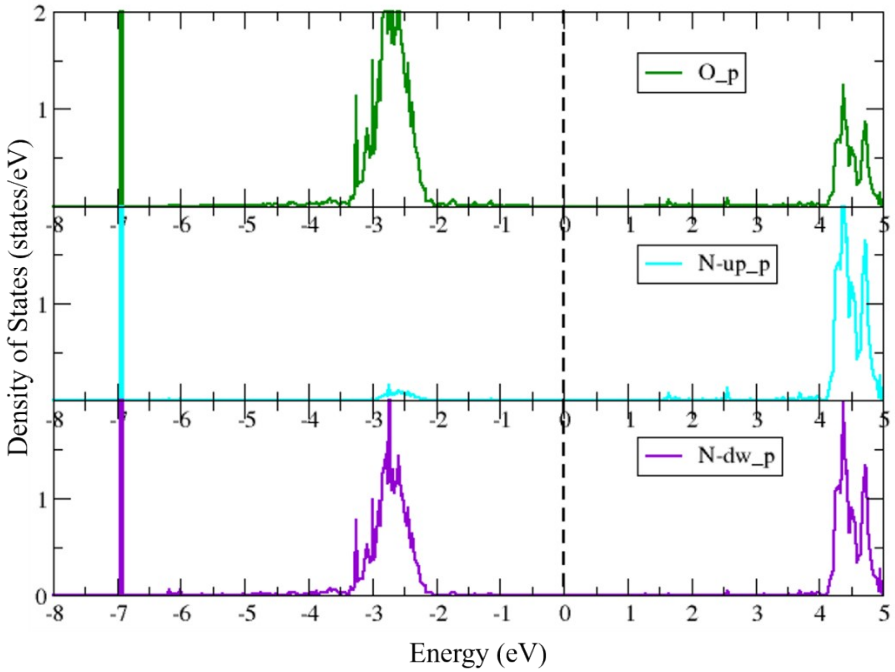

Figure S3, Projected Density of States for N_2O molecule adsorbed on Ti_{5c} site with N down configuration on TiO_2 Rutile (110) surface.

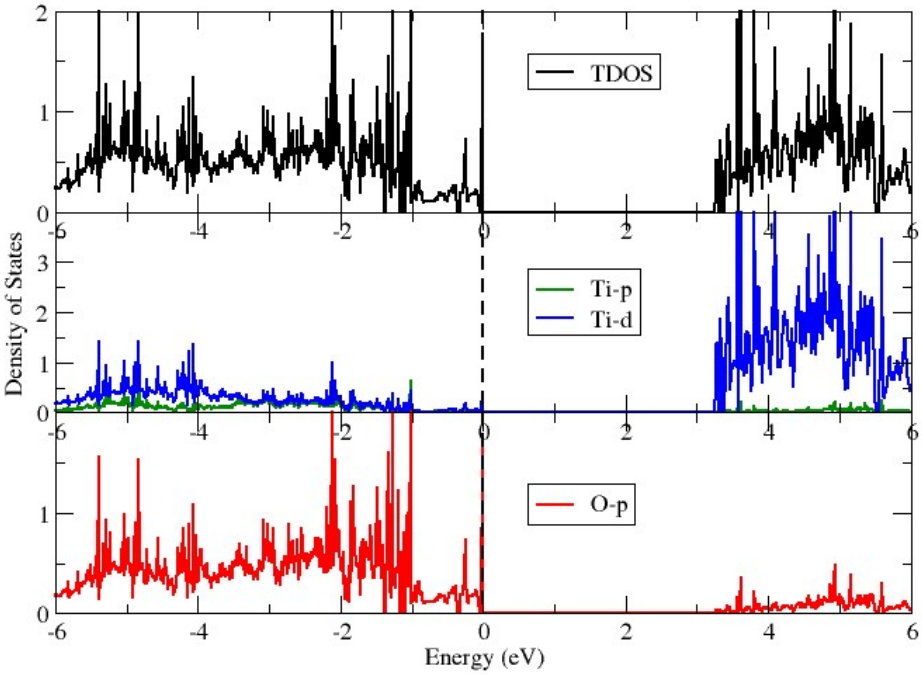

Figure S4, Projected density of states for pure Rutile TiO_2 (110) surface calculated by Hybrid density functional theory (HSE06) calculations with the bandgap of about 3.2 eV. Since the experimental bandgap of Rutile TiO_2 is 3.0 eV, here HSE06 functional slightly overestimated the bandgap. Most of the states are from O-2p and Ti-3d orbitals for valence and conduction bands, respectively.

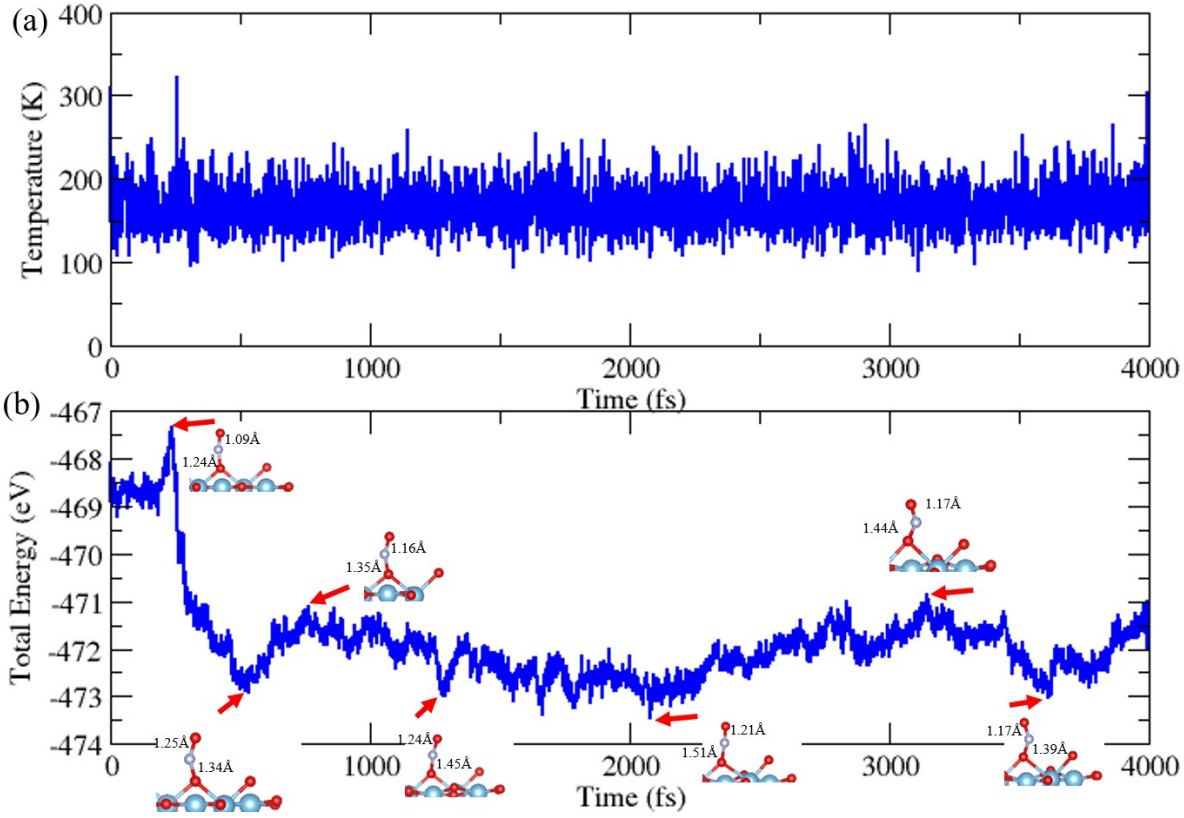

Figure S5, AIMD simulation for NO adsorbed TiO_2. The bond length of the NO molecule and its distance from the surface is higher in lower total energy, and it is lower in higher total energy.