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

Supplementary Information

NO adsorption and diffusion on hydroxylated rutile TiO_2(110)

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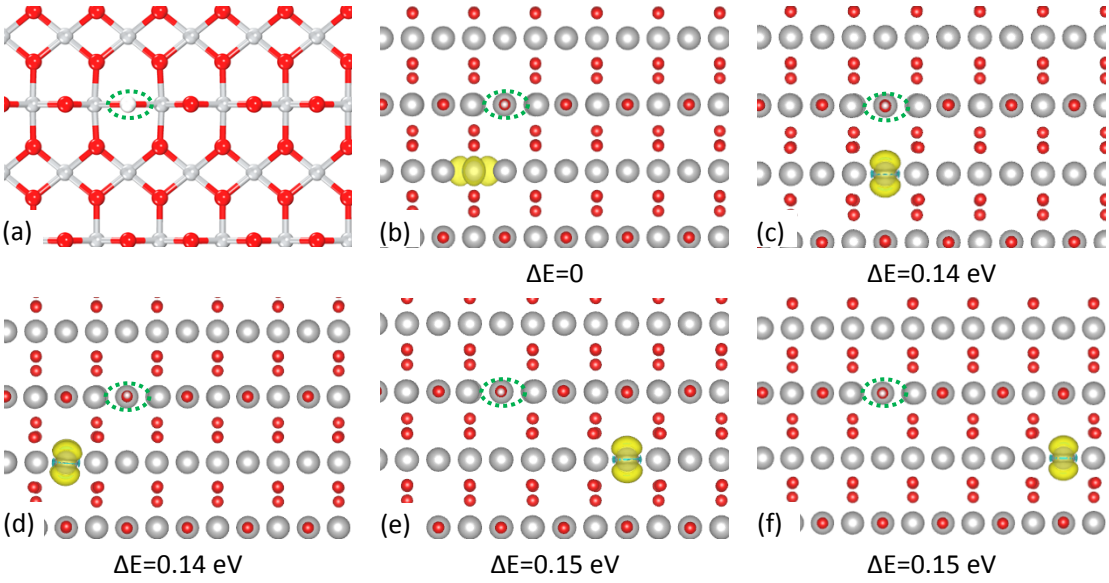

Fig. S1 Calculated structures of (a) the hydroxylated rutile TiO_2(110) surface and (b)-(f) the corresponding contour diagrams of the excess electron being localized at different Ti atoms in the subsurface (b) or on the surface (c-f).

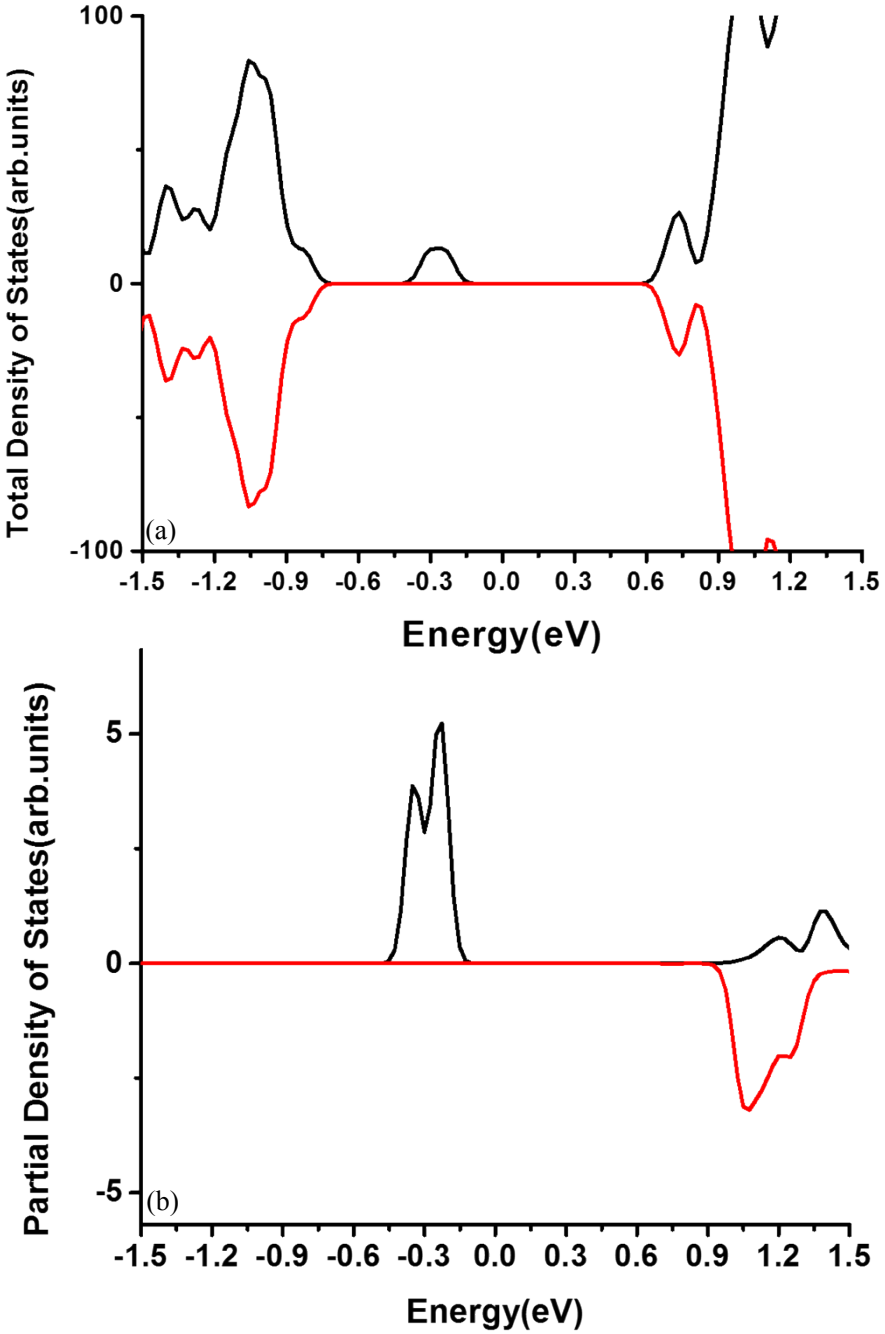

Fig. S2 Calculated total density of states of (a) NO adsorbed on the hydroxylated rutile TiO_2(110) surface, and (b) partial density of states of adsorbed NO.

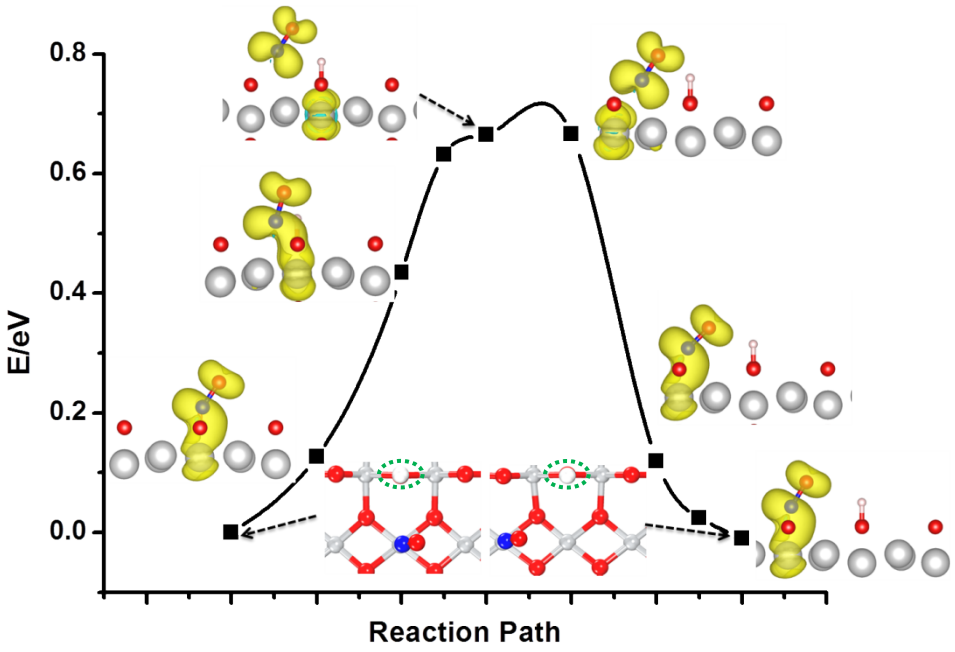

Fig. S3 Calculated energy profile of NO diffusion through Pathway III.