Electronic Supplementary Material (ESI) for Environmental Science: Nano.

N-doped TiO_2 anatase nanoparticle as a highly sensitive gas sensor for NO_2 detection: Insights from DFT computations

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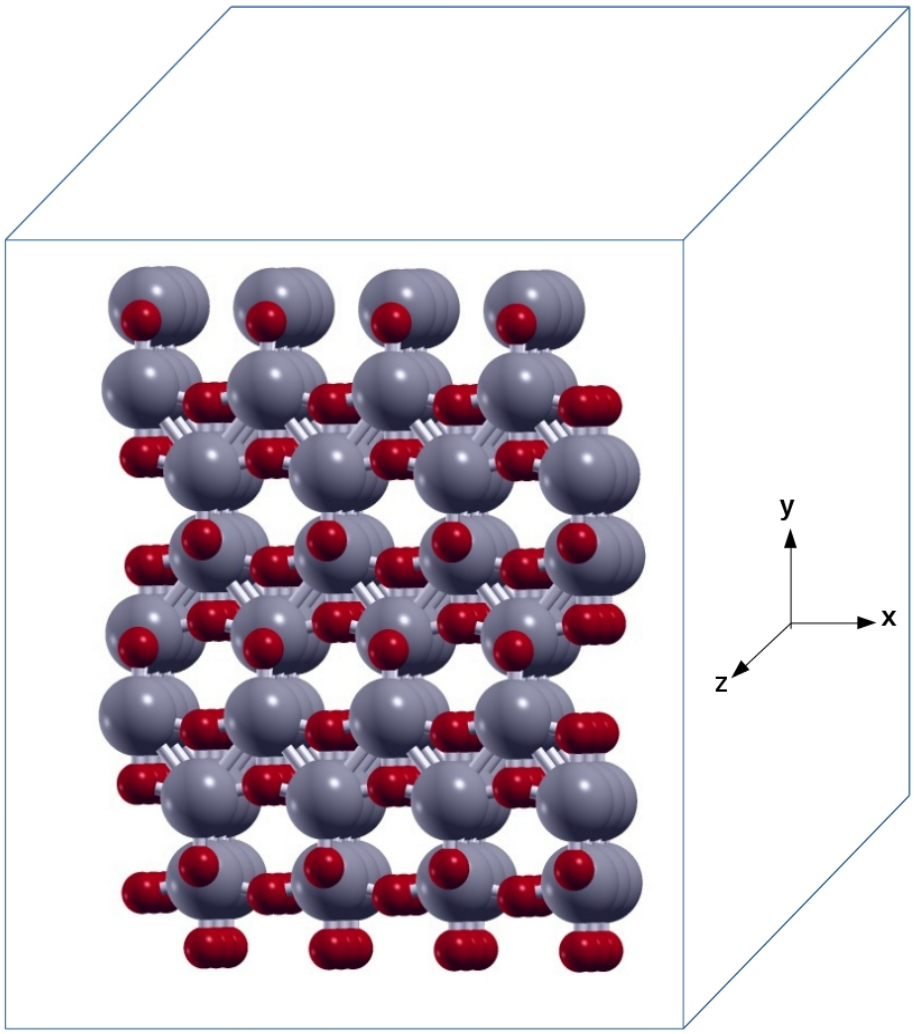

Figure S1. Representation of 3×2×1 supercell of the TiO_2 anatase constructed from the TiO_2 unit cells along x, y and z directions. The grey and blue balls denote titanium and nitrogen atoms, respectively.

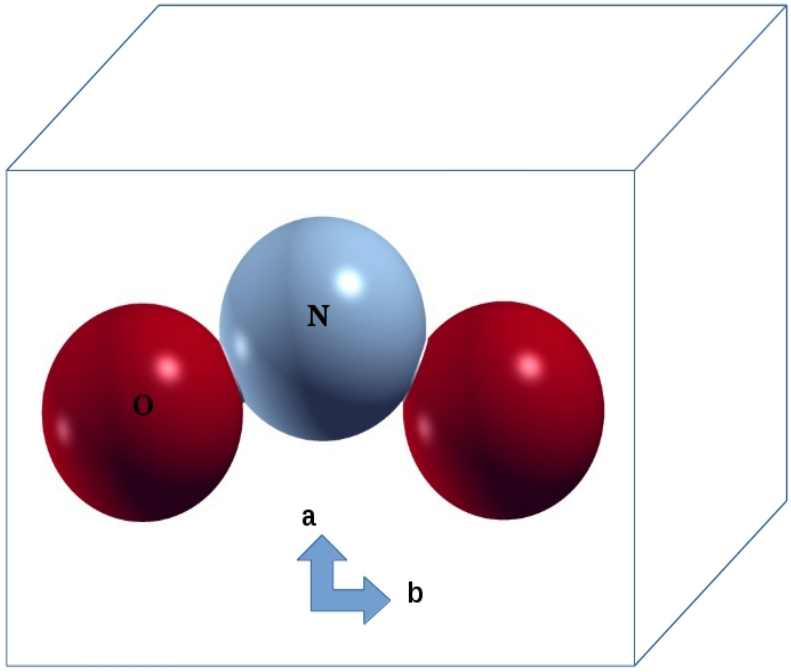

Figure S2. Schematic representation of the NO_2 molecule structure located in a large cubic supercell. The red and blue balls denote oxygen and nitrogen atoms, respectively.

NO_2 adsorption on the Ti-5f site (Bridging configuration)

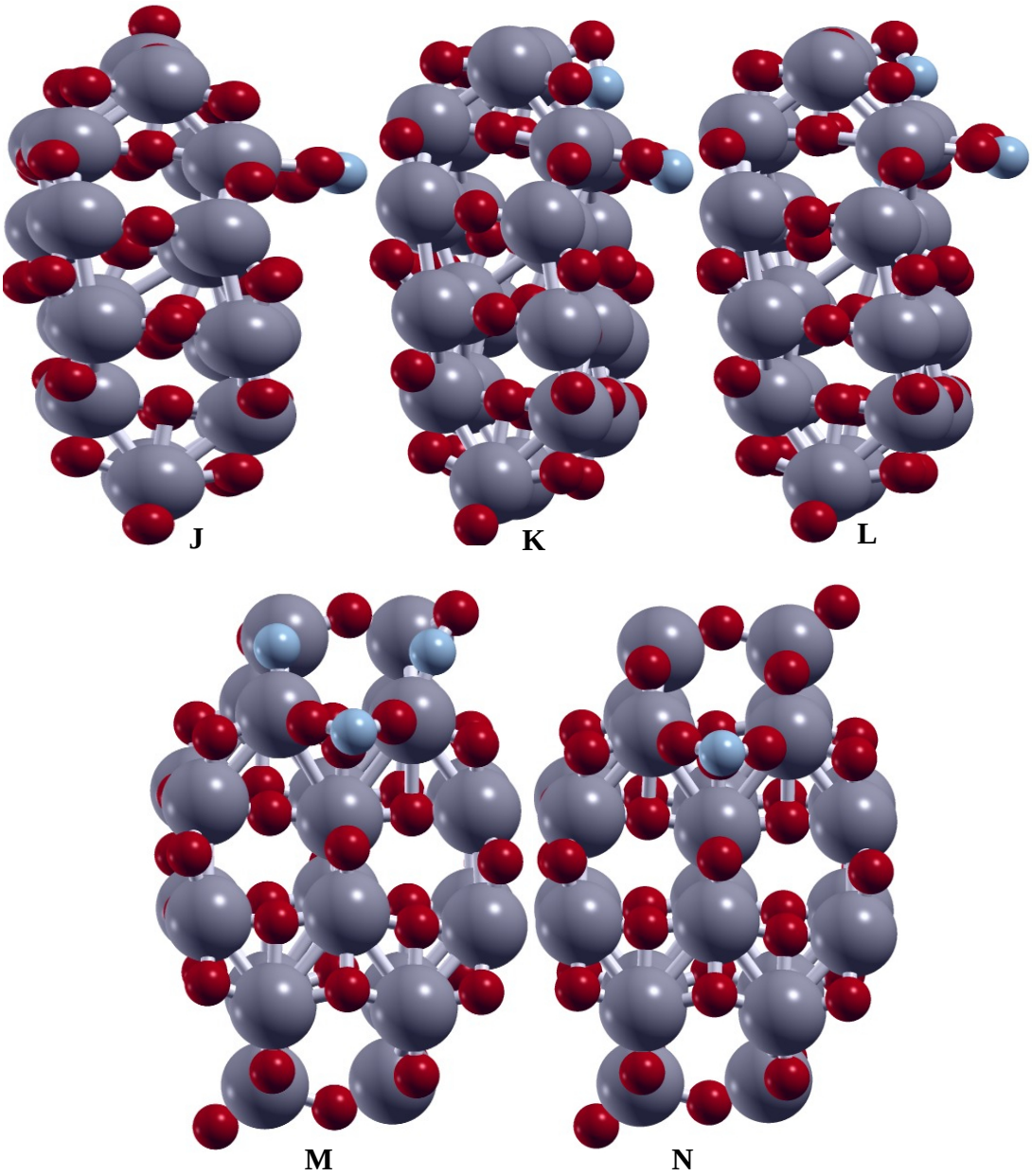

Figure S3. Optimized structures of the NO_2 molecule adsorbed on the TiO_2 anatase nanoparticles with nitrogen atom of the NO_2 molecule positioned towards the fivefold coordinated titanium atom of the nanoparticle.

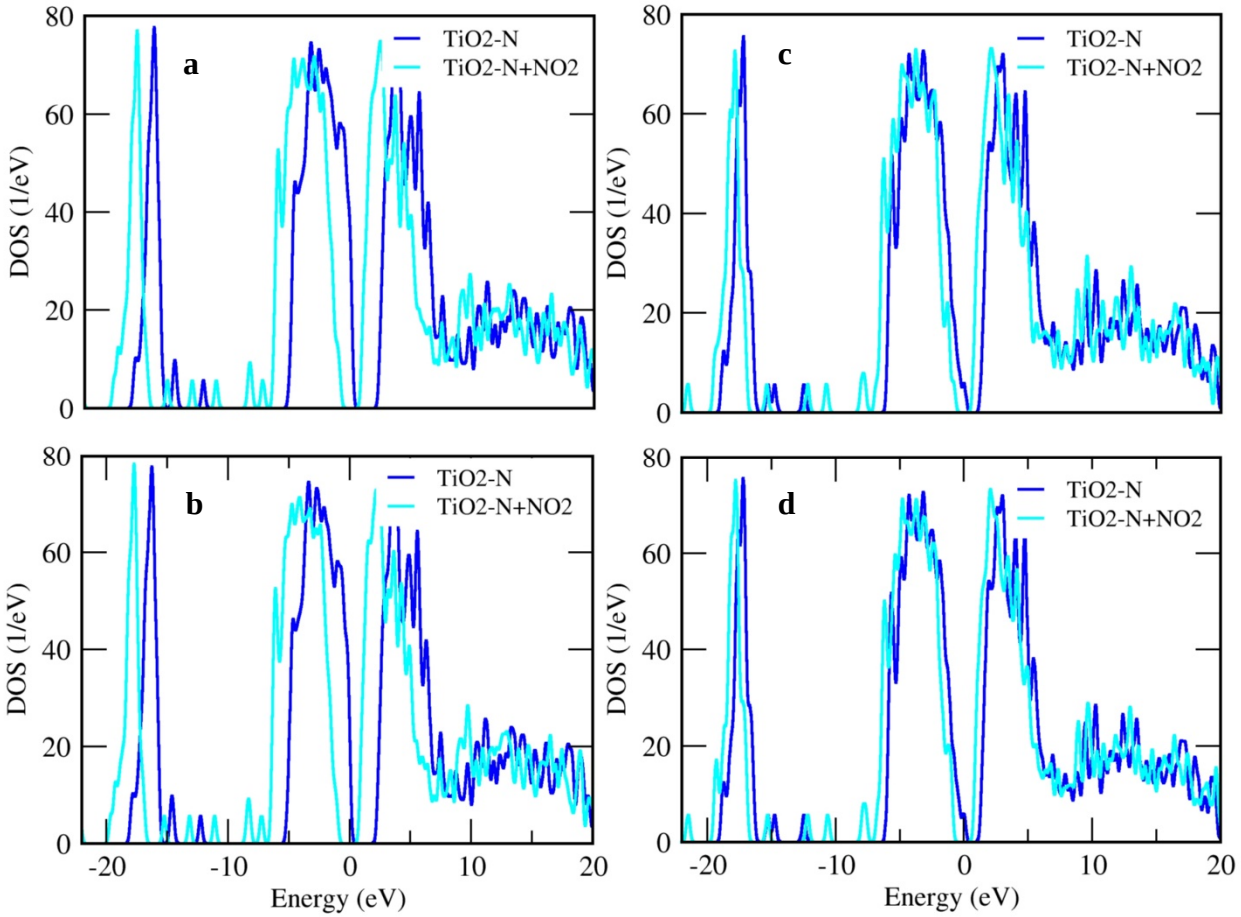

Figure S4. The total density of states (TDOS) of the NO_2 molecule adsorbed on the dangling oxygen site of the TiO_2 nanoparticle (the structures are shown in Figure 5). (a) Complex A; (b) Complex B; (c) Complex C; (d) Complex D. The Fermi level is set to 0 eV.

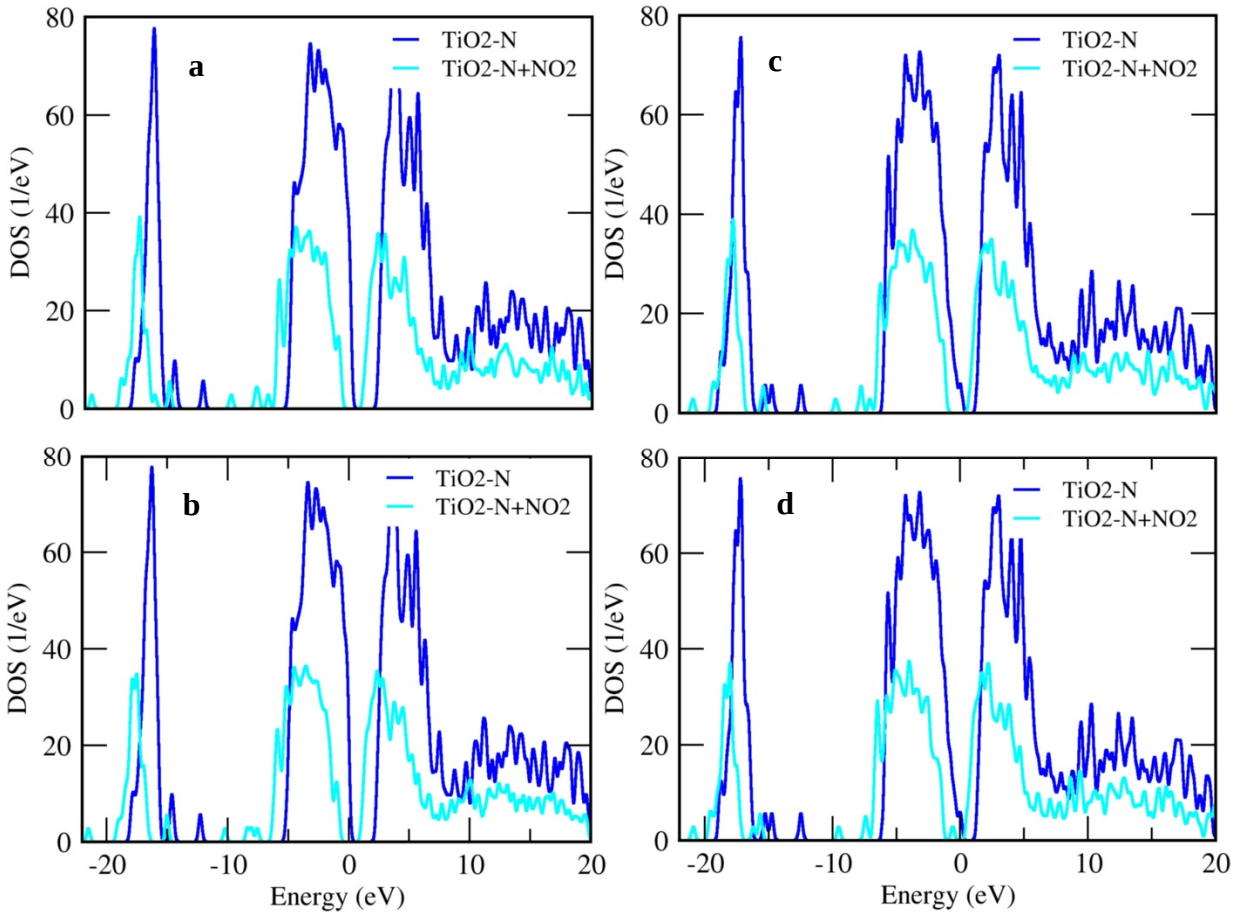

Figure S5. The total density of states (TDOS) of the NO_2 molecule adsorbed on the doped nitrogen site of the TiO_2 nanoparticle. (a) Complex F; (b) Complex G; (c) Complex H; (d) Complex I (the structures are shown in Figure 5). The Fermi level is set to 0 eV.

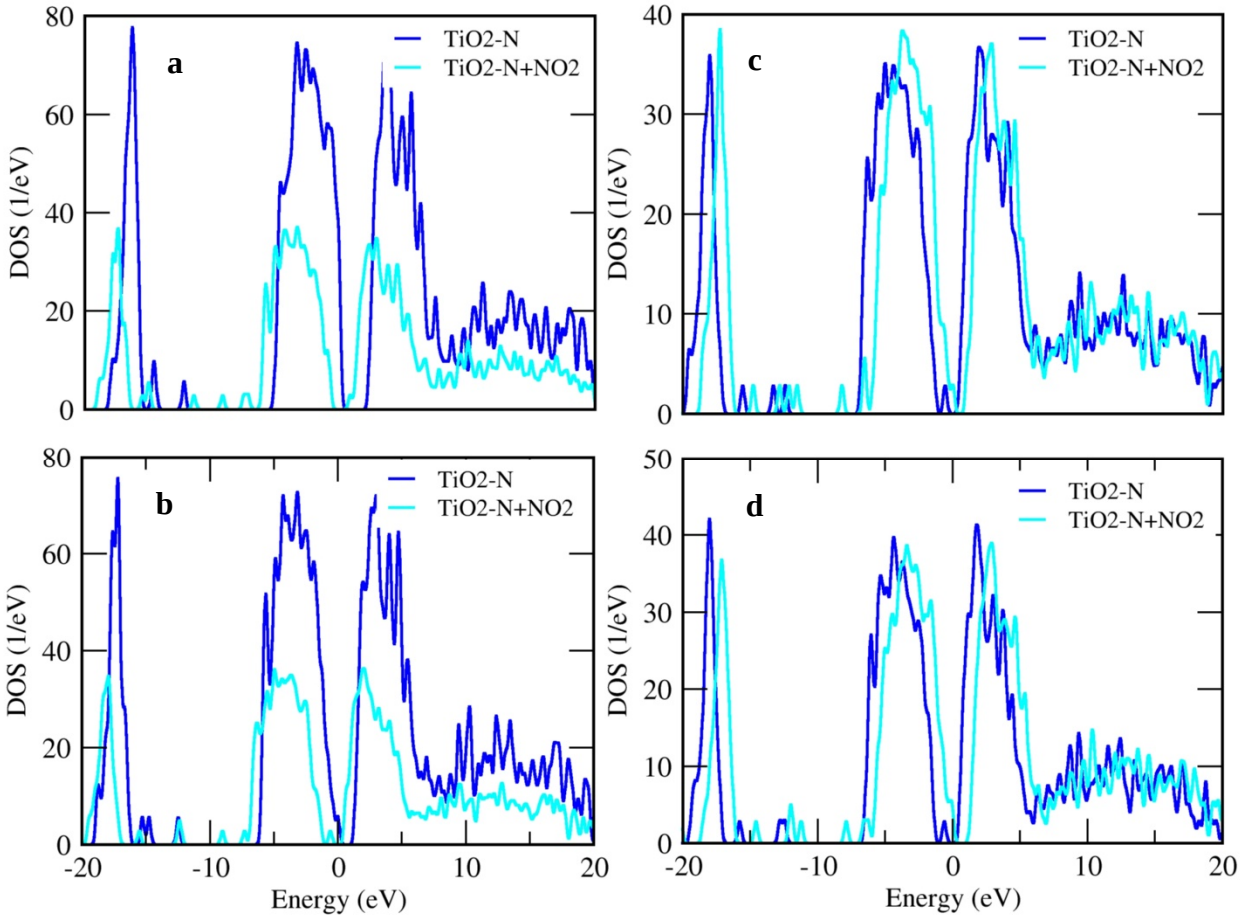

Figure S6. The total density of states (TDOS) of / the NO_2 molecule adsorbed on the fivefold coordinated titanium site of the TiO_2 nanoparticle. (a) Complex J; (b) Complex K; (c) Complex L; (d) Complex M. The Fermi level is set to 0 eV.

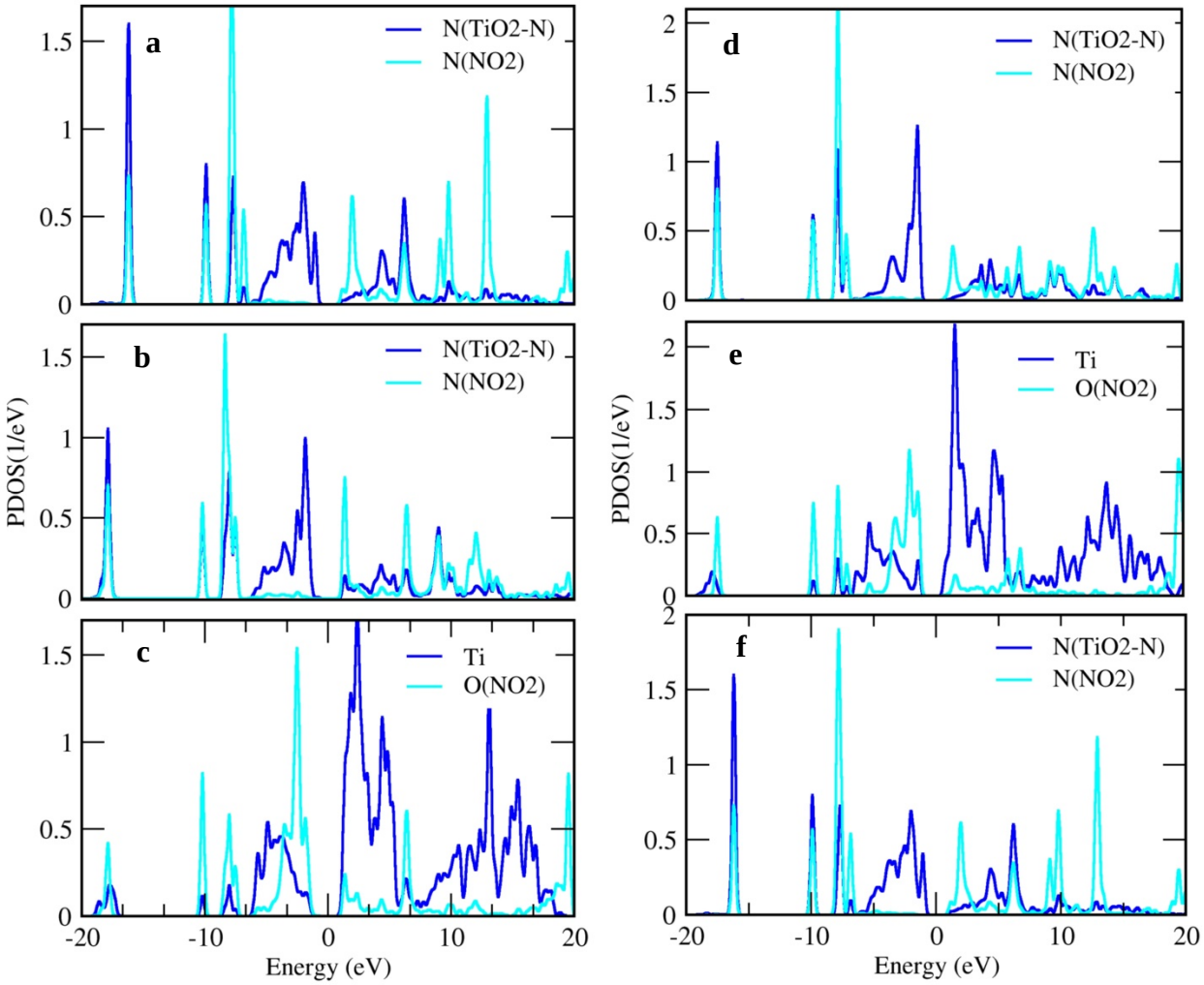

Figure S7. The projected density of states (PDOS) of the NO_2 molecule adsorbed on the doped nitrogen site of TiO_2 anatase nanoparticle. (a) Complex F; (b) Complex G; (c) Complex G; (d) Complex H; (e) Complex H; (f) Complex I.

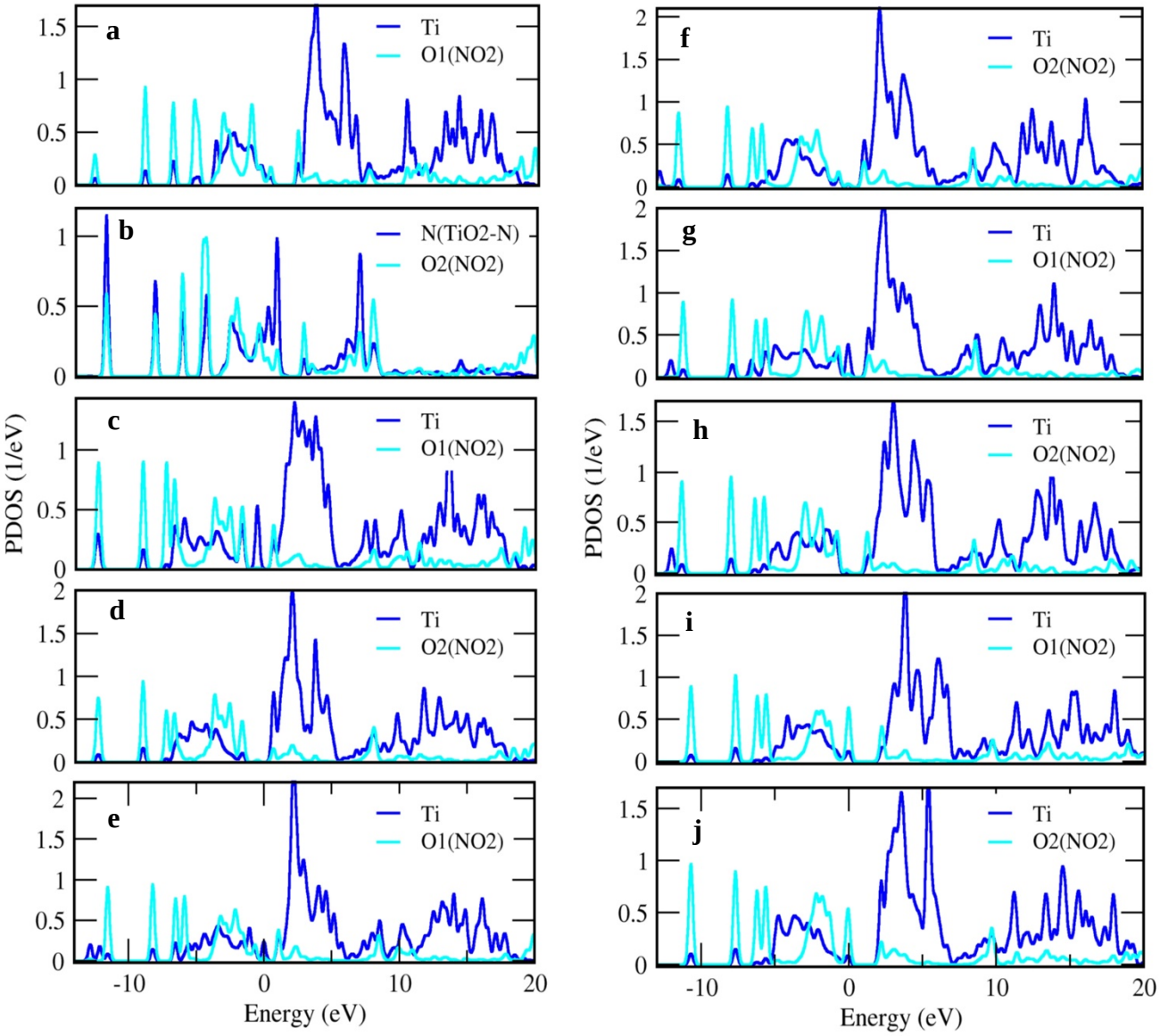

Figure S8. The projected density of states (PDOS) of the NO_2 molecule adsorbed on the fivefold coordinated titanium site of TiO_2 nanoparticle, (a) Complex J; (b) Complex J; (c) Complex K; (d) Complex K; (e) Complex L; (f) Complex L; (g) Complex M; (h) Complex M; (i) Complex N; (j) Complex N.

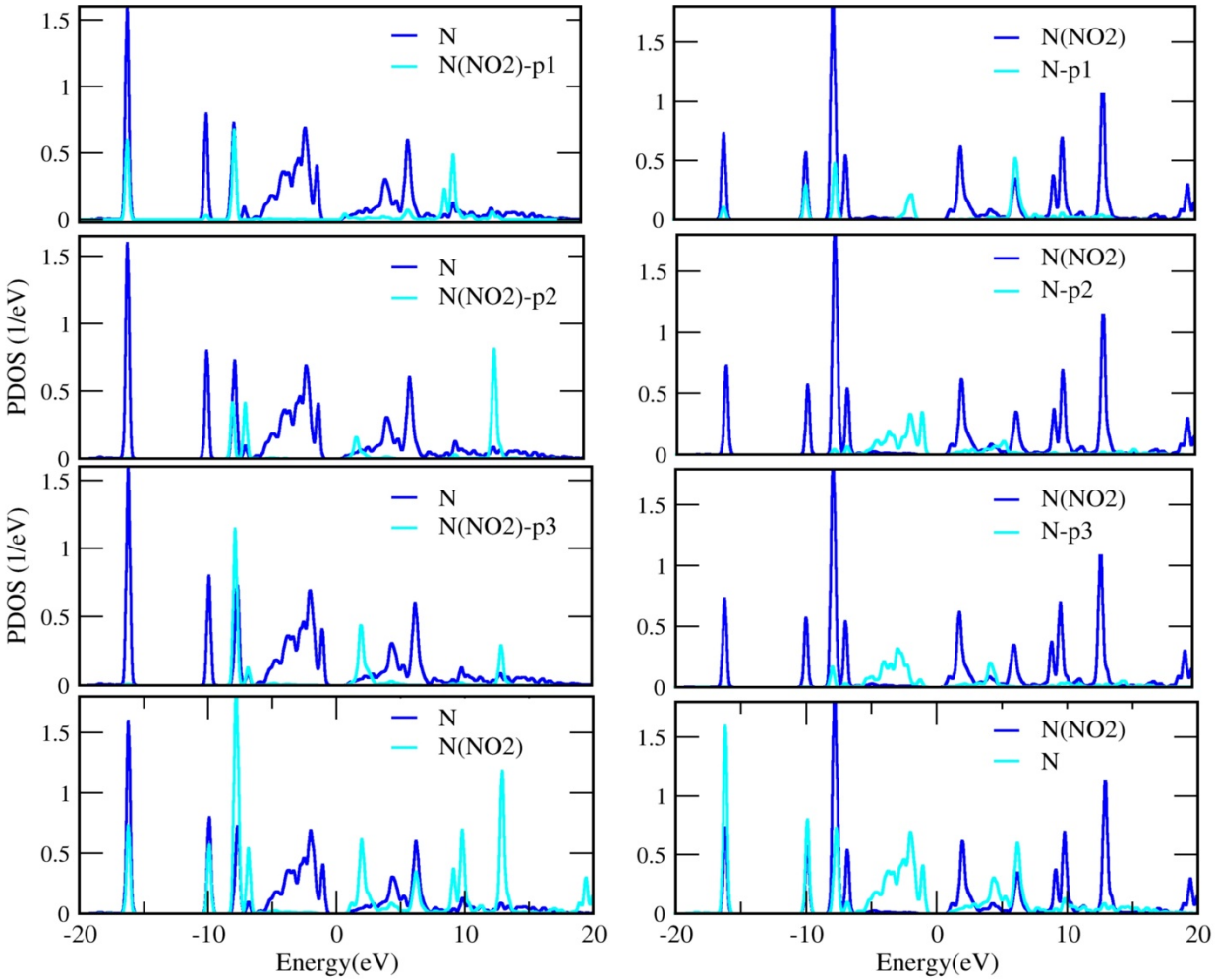

Figure S9. The projected density of states (PDOS) for two nitrogen atoms forming chemical bond at the interface and their three p orbitals for complex F (first column represents the PDOSs of the nitrogen atom of nanoparticle and different p orbitals of the nitrogen atom of NO_2 molecule, whereas the second column tells the PDOSs of the nitrogen atom of NO_2 molecule and p orbitals of the nitrogen atom of nanoparticle).

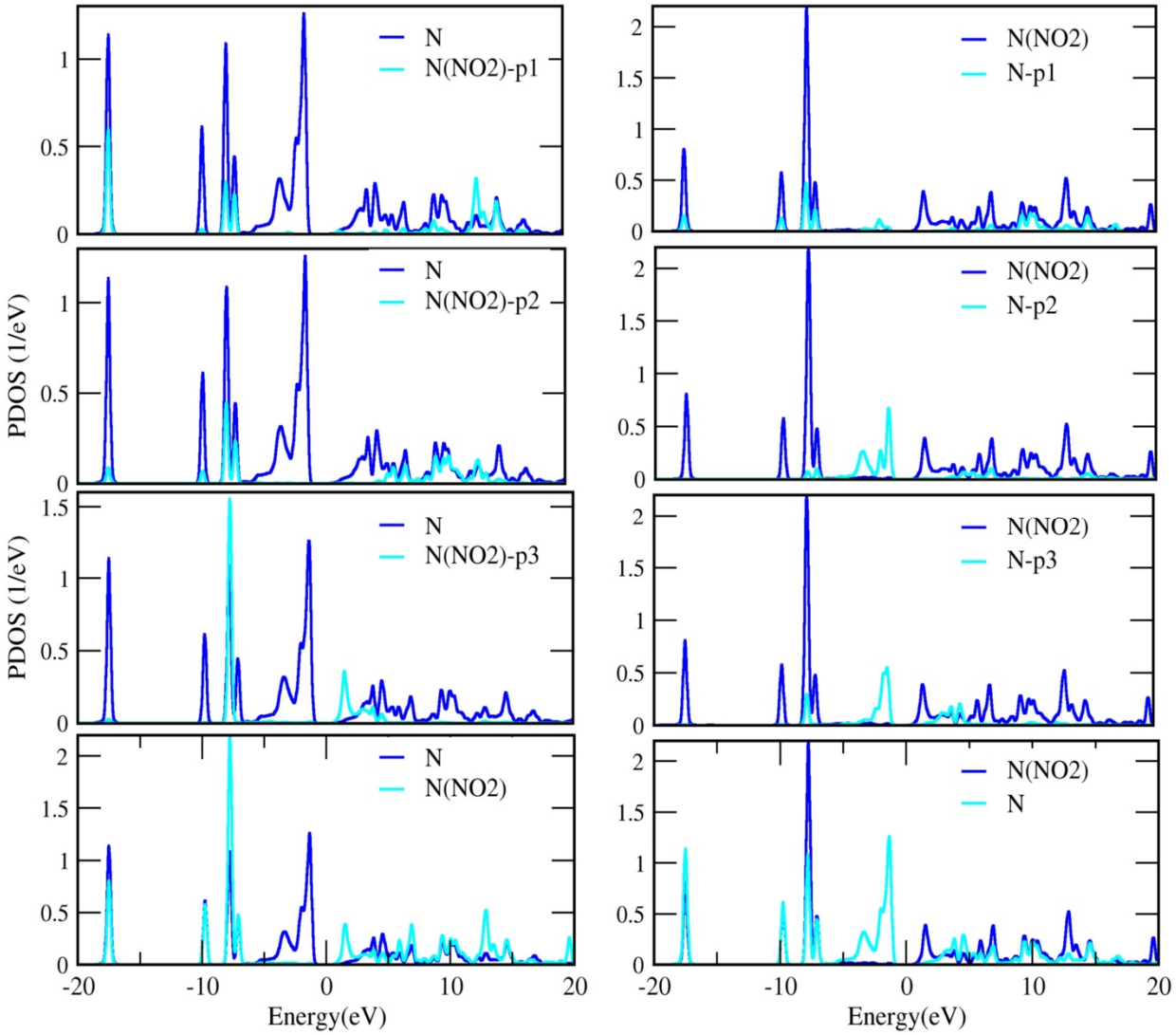

Figure S10. The projected density of states (PDOS) for two nitrogen atoms forming chemical bonds at the interface and their three p orbitals for complex H (the first and second columns represent the PDOSs of the nitrogen atoms of the NO_2 molecule and TiO_2 nanoparticle and their pertaining p orbitals).

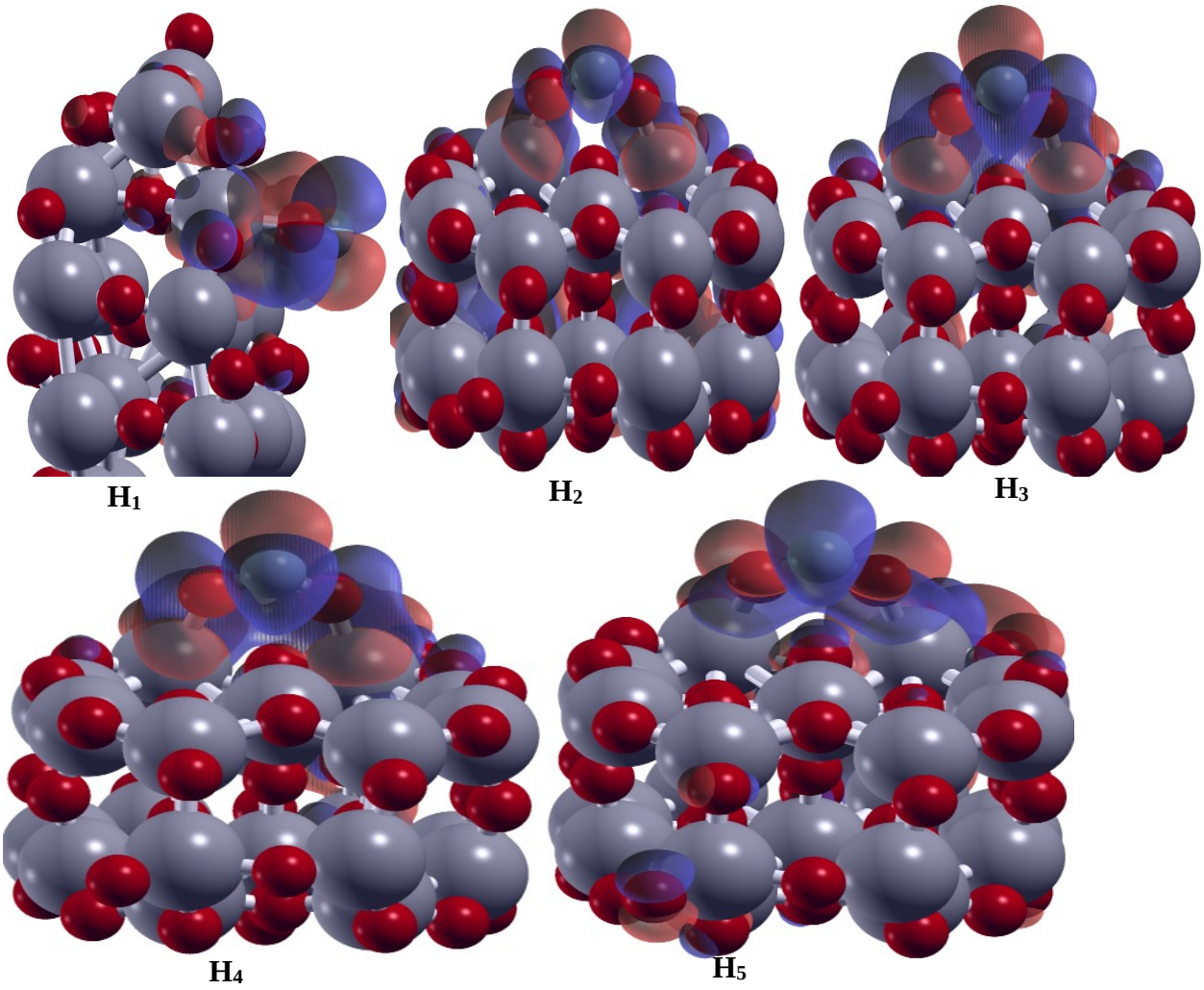

Figure S11. Isodensity surfaces of the highest occupied molecular orbitals (HOMO) for the NO_2 molecule adsorbed on the fivefold coordinated titanium sites of the TiO_2 nanoparticles. (H_1) Complex J; (H_2) Complex K; (H_3) Complex L; (H_4) Complex M; (H_5) Complex N.

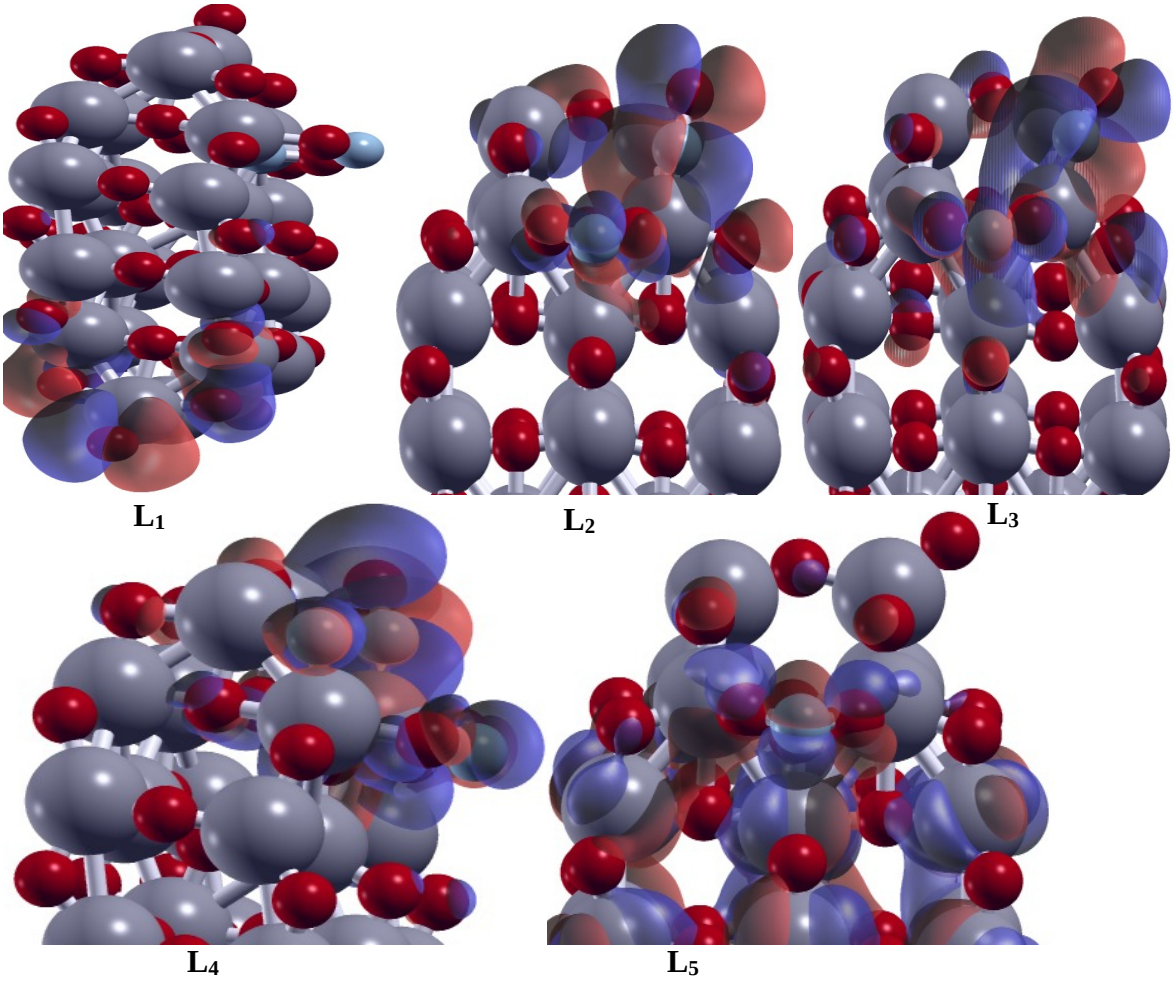

Figure S12. Isodensity surfaces of lowest unoccupied molecular orbitals (LUMO) for the NO_2 molecule adsorbed on the O_D and doped nitrogen sites of the TiO_2 nanoparticles. (L_1) Complex J; (L_2) Complex K; (L_3) Complex L; (L_4) Complex M; (L_5) Complex N.