1	Facet-dependent photocatalytic decomposition of N_2O on the anatase	
2	TiO ₂ : A DFT study	
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Supplementary computational details of the relative level of CBM (Conduction Band
 Minimum) for (101) facets and (001) facets

We calculated the local potential along the z-axis of the (101) facets and (001) facets which are shown in Figure S1 and Figure S2, respectively. We selected a point deep in the vacuum (18 Å) as the reference energy for (101) facets and (001) facets. In this point, the local potential are 3.29 eV and 2.81 eV, respectively. The difference of electrostatic potential is 0.48 eV. The original CBM for (101) facets and (001) facets are -0.61 eV and -0.38 eV, respectively. Therefore, the CBM for (001) facets is 0.71 eV higher than that for (101) facets.

1 2. Supplementary computational details of crystal orbital Hamiltonian population (COHP)

2 The bonding analysis have been performed through the use of the crystal orbital Hamiltonian 3 population (COHP)^{1,2} by the Lobster code^{3,4}. The COHP can measure the magnitude and sign of 4 the bond order energy overlap between atomic orbitals located on different atoms. It can 5 determine the bonding or the antibonding nature of orbital fragments. It can also measure the 6 interaction strength between two atomic orbitals.

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8 References

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1 3. Supplementary Figures







Fig. S2 The local potential along the z-axis of the (001) facets





2 Fig. S3 Relative energy diagram for the removal of O⁻ on (101) facets (O⁻ react with another O⁻)





3 Fig. S4 Relative energy diagram for the removal of O⁻ on (101) facets (O⁻ react with N₂O)



2 Fig. S5 Relative energy diagram for the removal of O⁻ on (001) facets (O⁻ react with another O⁻)



3 Fig. S6 Relative energy diagram for the removal of O⁻ on (001) facets (O⁻ react with N₂O)



Fig. S7 -COHP between Ti-O for (001) and (101) facets. Fermi level is set to zero.



Fig. S8 -COHP between Ti-O⁻ for (001) and (101) facets. Fermi level is set to zero.



1 4. Supplementary Figures

Facets	State of O	ICOHP value
	0	-2.61
101	O-	-3.68
	O ²⁻	-5.49
	0	-3.61
001	O [.]	-3.96
	O ²⁻	-5.59

2 Table S1 The integrated ICOHP value of O-Ti on different facets