

Appendix A: Supporting information (SI):

**Oxygen vacancies enhanced photocatalytic removal of
NO over N-doped TiO₂ catalyst**

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SI.1 Calculation of energy band

The E_g value was calculated by the Graetzel relation. The Graetzel relation:

$$E_g = 1240/\lambda_g \text{ (eV)} \quad (\lambda_g : \text{Absorption wavelength threshold}).$$

SI.2 XPS of TiO₂ sample

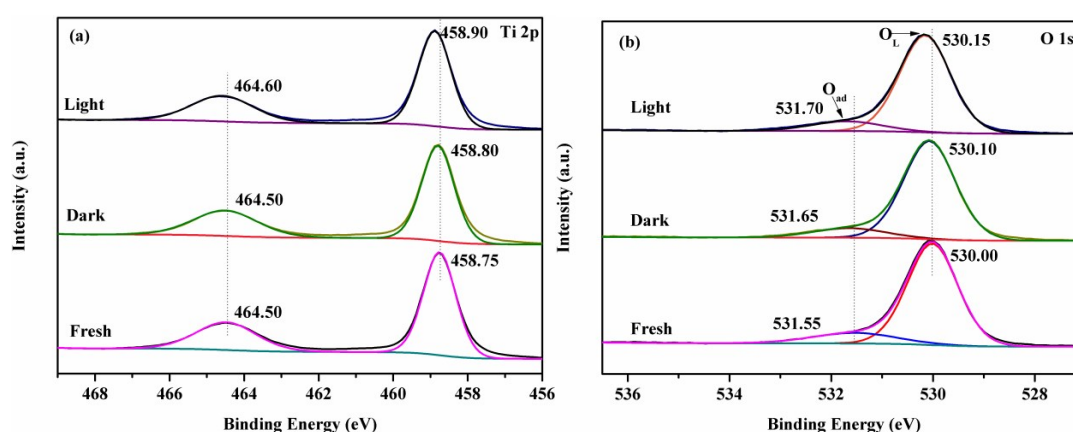


Fig.S1. High-resolution XPS spectra for TiO₂ sample of fresh, after reacted in dark or under visible irradiation: (a) Ti 2p and (b) O 1s.

Table S1 The High-resolution XPS spectra area for TiO₂ sample of O 1s.

Name	Fresh sample(Area (P) CPS.eV)	Reacted in dark (Area (P) CPS.eV)	Reacted in light(Area (P) CPS.eV)
O _(L)	299486	296418	290087
O _(ad)	51918	40309	40358

The electron binding energy for Ti2p and O1s of TiO₂ sample exhibited an increasing tendency from fresh to after reacted in dark and then reacted under visible light irradiation, suggesting that TiO₂ sample could be oxidized by O₂ gas and then O₂ gas got electrons forming $\cdot\text{O}_2^-$ species ($\text{O}_2 + e^- \rightarrow \cdot\text{O}_2^-$). In addition, as shown in table 1, the peak at about 530.15 eV was assigned to the lattice oxygen species.

SI.3 O₂-TPD of TiO₂ sample

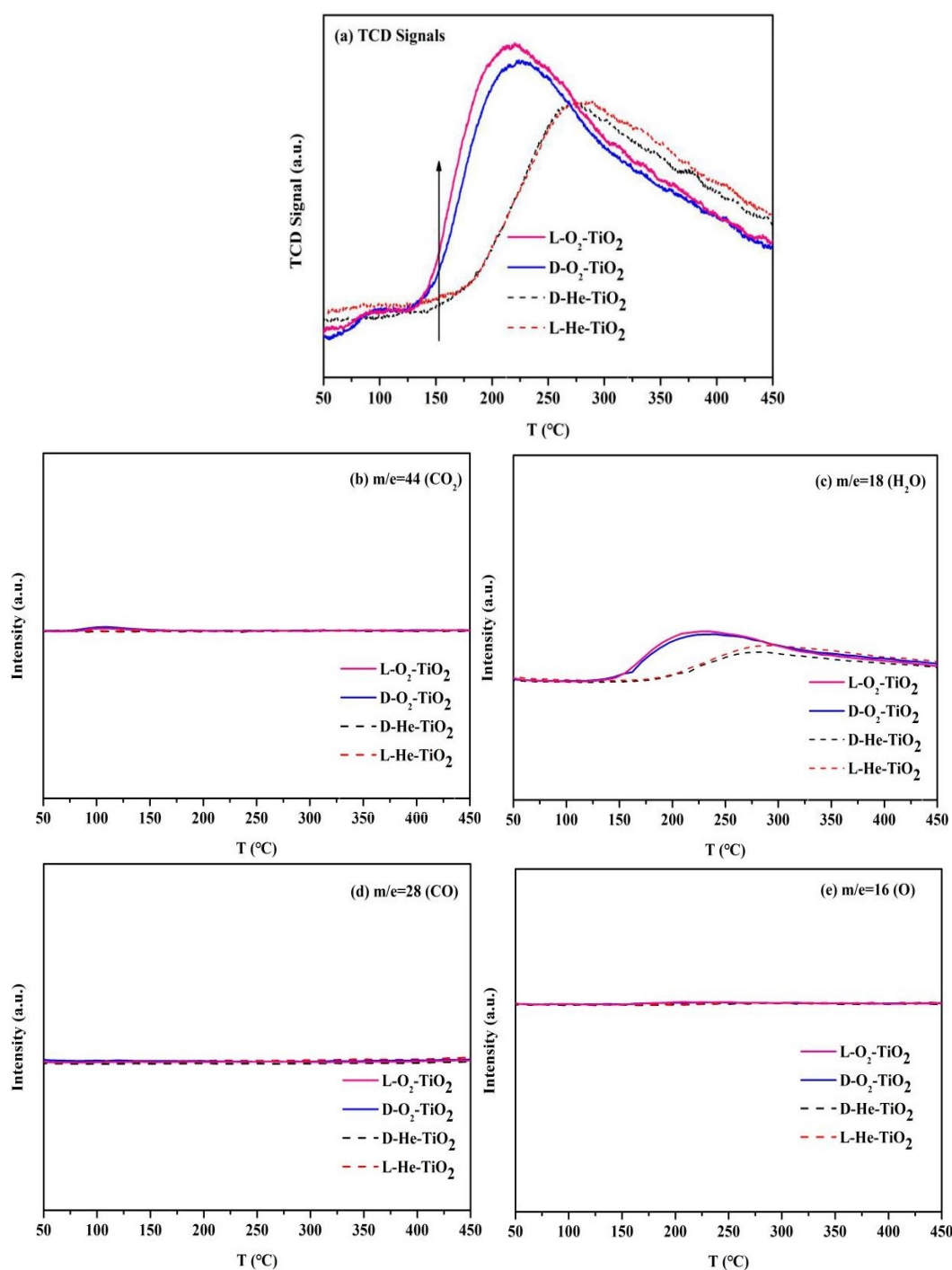


Fig. S2. The O₂-TPD-MS results of TiO₂ catalyst after pre-adsorb O₂ and He under visible light or not. (catalyst dosage: 0.1 g、He was injected during heating).

The O₂-TPD testing graph of TiO₂ samples showed a signal peak at 225 °C, ascribed to the production of H₂O species in combination with the mass spectrum result.

SI.4 Assignment hydroxyl of FT-IR spectra

Table S2 Assigned hydroxyl of FT-IR spectra of adsorbing NO or NO+O₂ over TiO₂ and N-TiO₂ samples under visible light irradiation, respectively.

Sample bands	Terminal-OH	Bridged isolated -OH	Single coordinated -OH	Bridged -OH	doubly coordinated -OH
N-TiO ₂ (NO)	3730	3700	3670		3475
N-TiO ₂ (NO+O ₂)	3732 3716		3679, 3652	3612	3470