

Supporting Information

Oxygen vacancies assist facet effect to modulate the microstructure of TiO₂ for efficient photocatalytic O₂ activation

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Tables and Figures

Table S1 Average pore size and BET specific surface area of the as-prepared samples.

Samples	Pore size (nm)	Specific surface area (m ² ·g ⁻¹)
T101	5.56	181.58
T001-V _O	19.12	54.76
T101-V _O	5.63	155.82

Table S2 Electrochemical impedance spectroscopy (EIS) parameter of the as-prepared samples.

Samples	R_s (Ohm)	R_{ct} (Ohm)	CPE
T101	35.05	109830	0.97
T001-V _O	41.15	100030	0.93
T101-V _O	38.22	51028	0.93

R_s is the series resistance, which represents the resistance generated by the electrolyte solution and circuit components; CPE is the constant phase element of capacitance corresponding to R_{ct} .

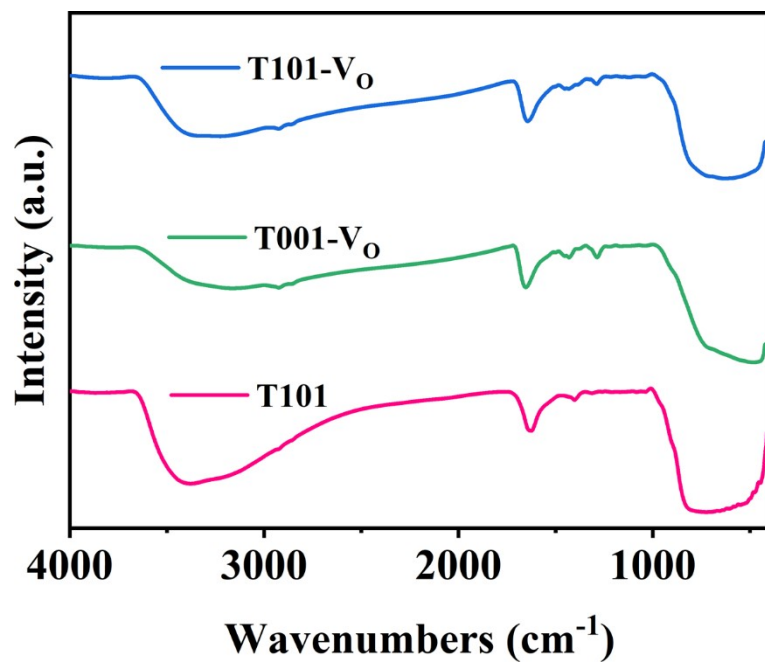


Fig. S1 FT-IR of the samples.

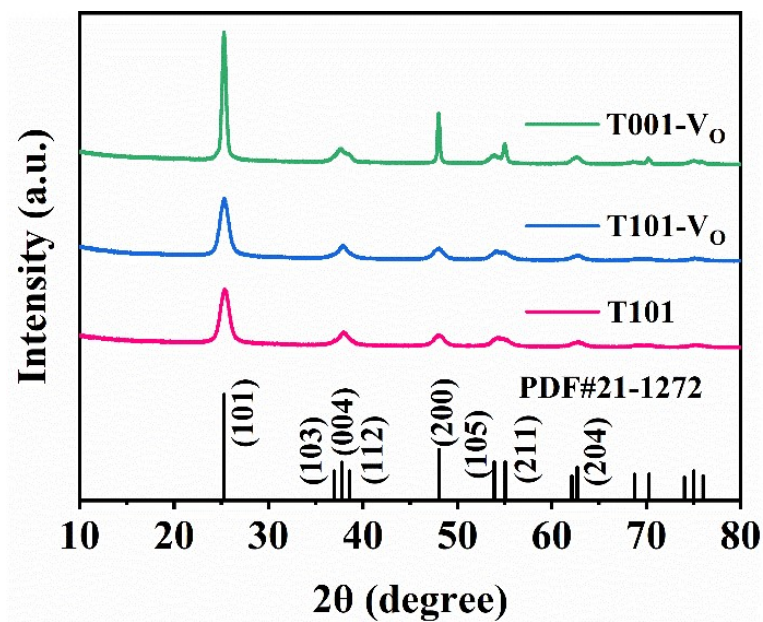


Fig. S2 XRD patterns of the samples.

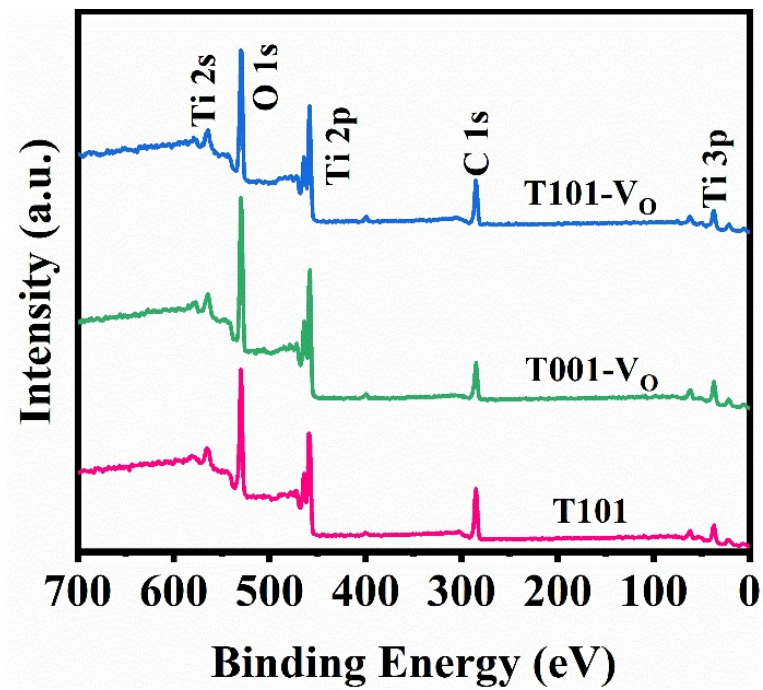


Fig. S3 XPS survey spectra of the samples.

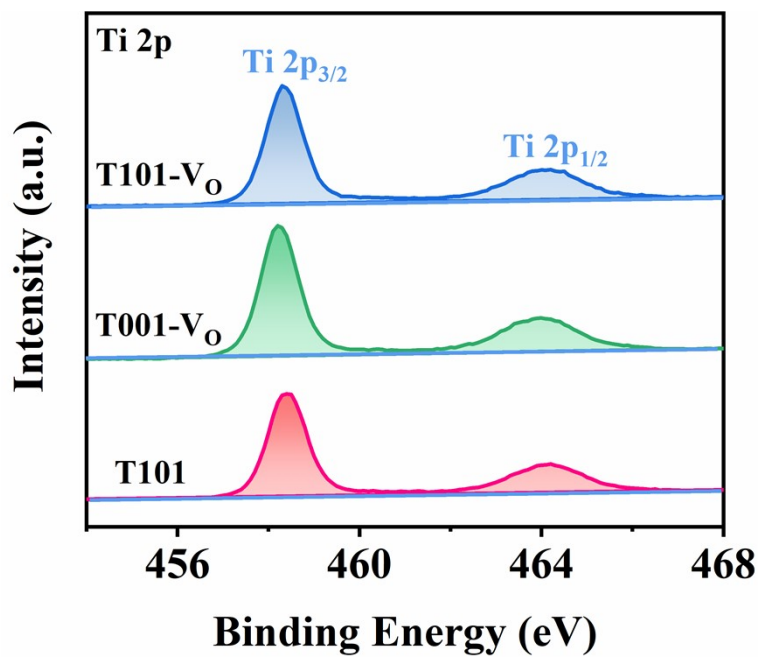


Fig. S4 The Ti 2p high resolution XPS spectra of the samples.

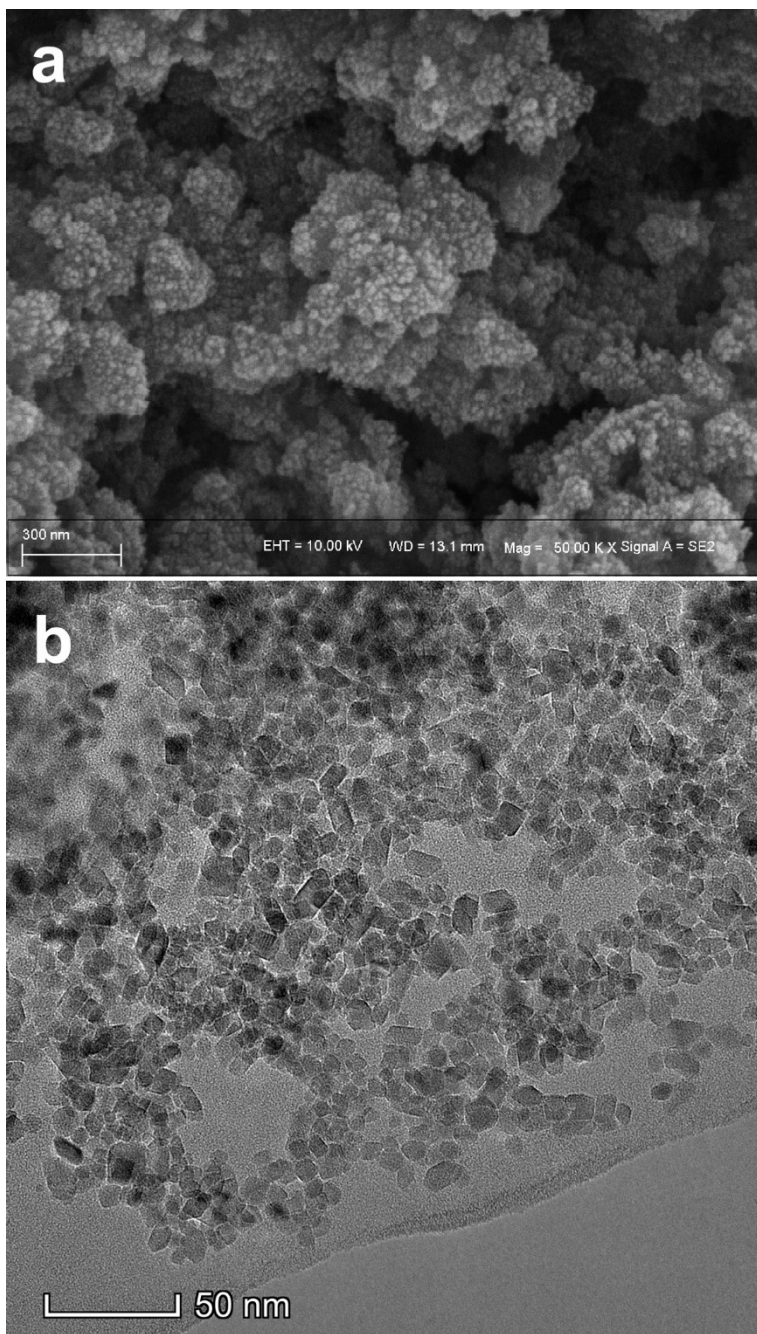


Fig. S5 (a) SEM image and (b) TEM image of T101.

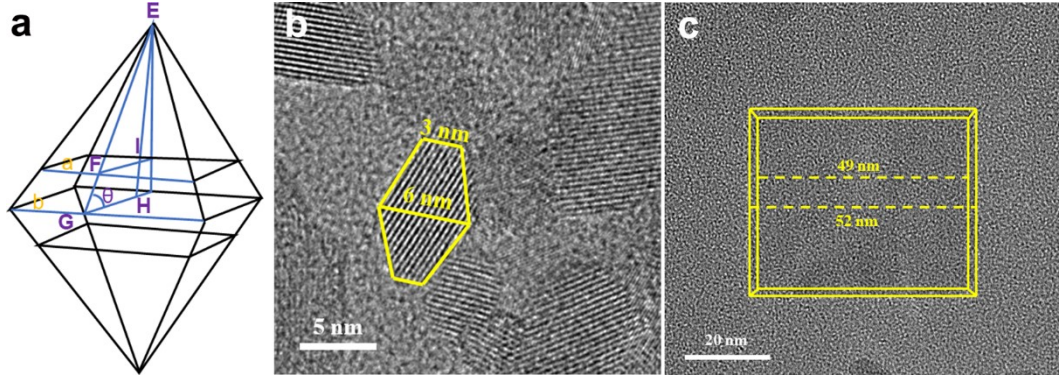


Fig. S6 (a) TiO₂ geometry configuration; TEM images of (b) T101-V_O and (c) T001-V_O.

The percentages of {001} and {101} in the TiO₂ nanocrystals were calculated by following similar methods reported in previous literature.^{1,2} Herein, θ is the theoretical value (68.3°) for the angle between the {001} and {101} facets of anatase. The length of a and b were obtained from the HR-TEM images.

$$\begin{aligned}
 \{001\}\% &= \frac{S_{001}}{S_{001} + S_{101}} \times 100\% \\
 &= \frac{2a^2}{2a^2 + 8\left(\frac{1}{2}EG \times b - \frac{1}{2}EF \times a\right)} \times 100\% \\
 &= \frac{a^2}{a^2 + 4\left(\frac{1}{2} \times \frac{1}{2}b \times \frac{1}{\cos\theta} \times b - \frac{1}{2} \times \frac{1}{2}a \times \frac{1}{\cos\theta} \times a\right)} \times 100\% \\
 &= \frac{\cos\theta}{\cos\theta + \frac{b^2}{a^2} - 1} \times 100\%
 \end{aligned}$$

Results:

T101-V_O: S_{001}=11%, S_{101}=89%; T001-V_O: S_{001}=76%, S_{101}=24%.

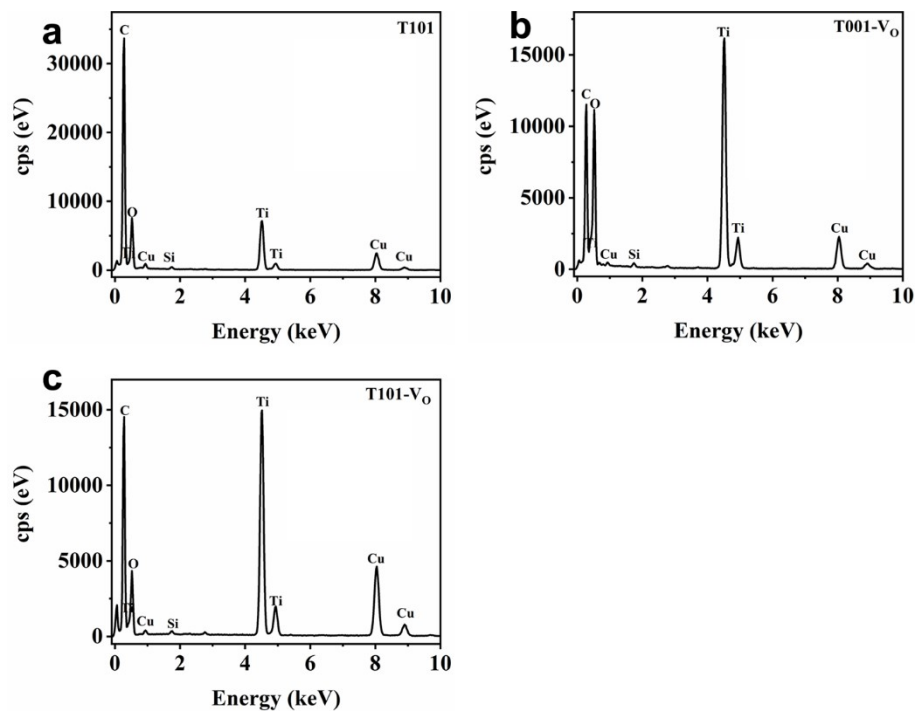


Fig. S7 TEM-EDS of (a) T101, (b) T001-V_O and (c) T101-V_O.

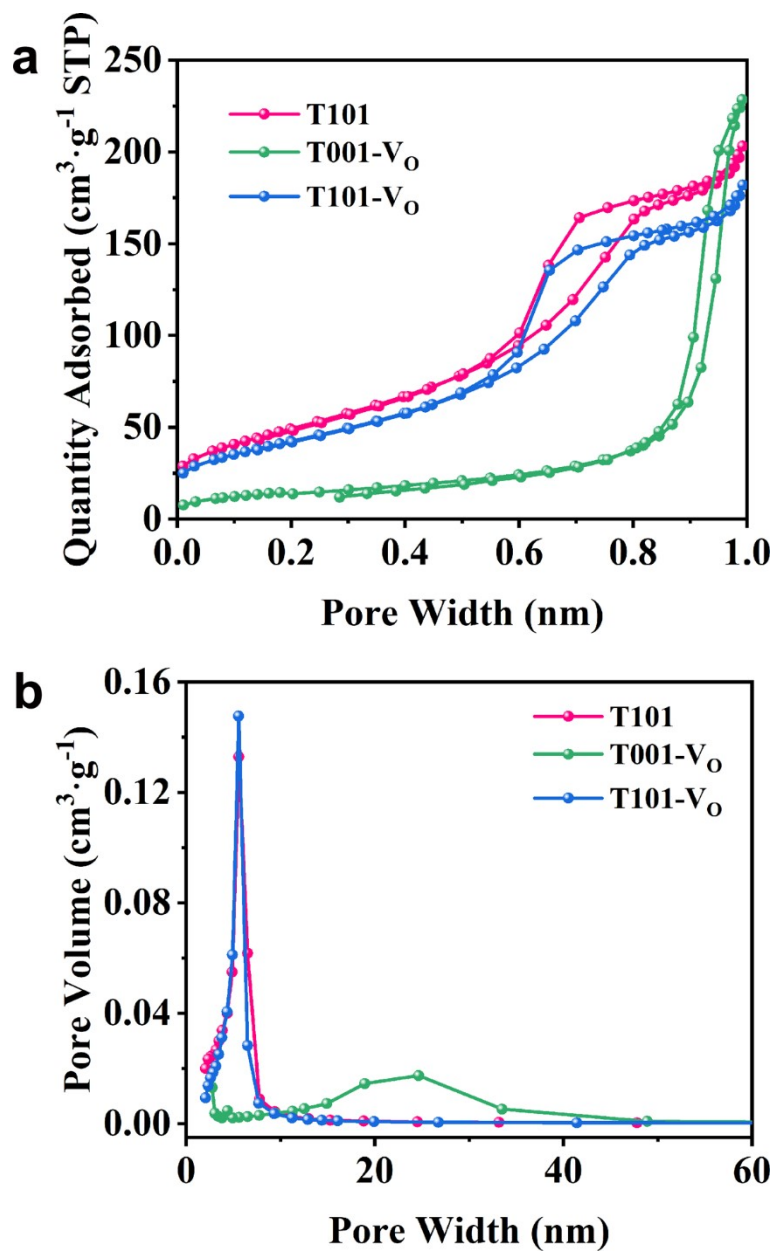


Fig. S8 (a) N₂ adsorption/desorption isotherms and (b) pore width of the samples.

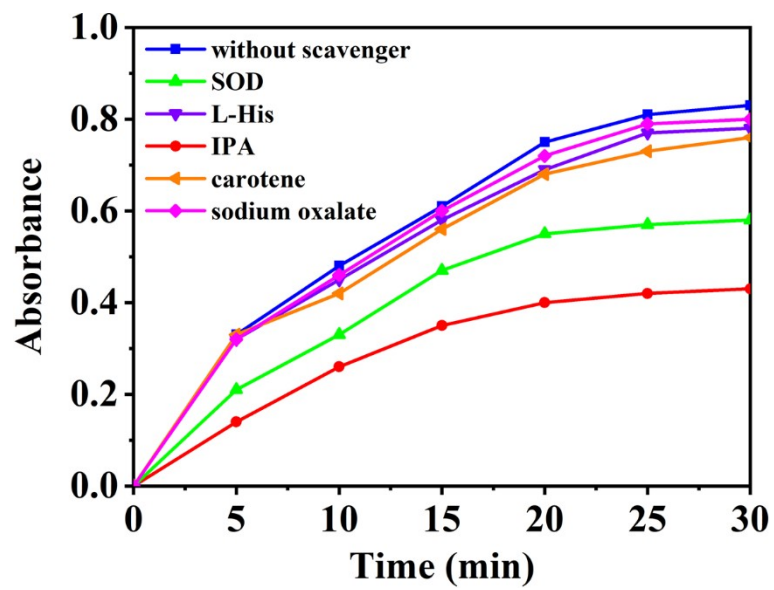


Fig. S9 Absorbance change over T101-V_O with different scavengers of TMB oxidation.

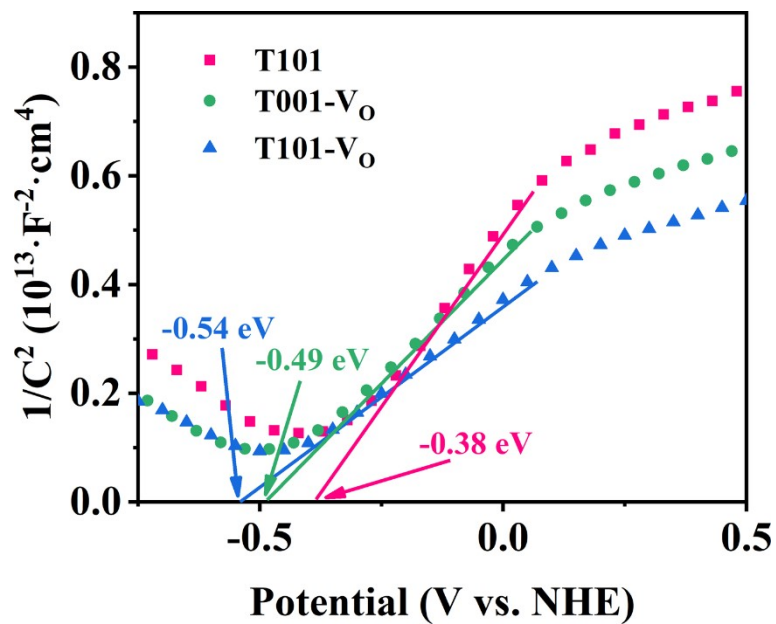


Fig. S10 Mott-Schottky plots of the samples.

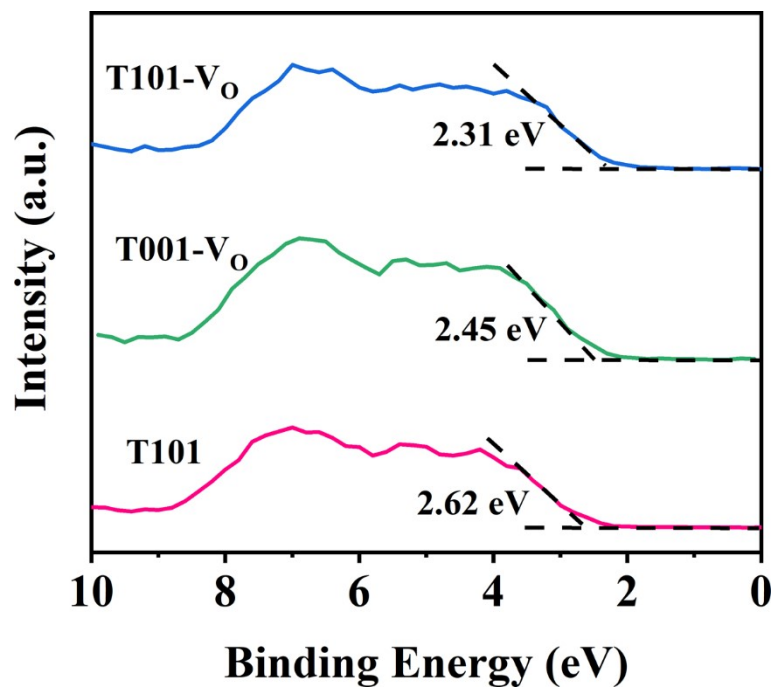


Fig. S11 Valence band of the samples.

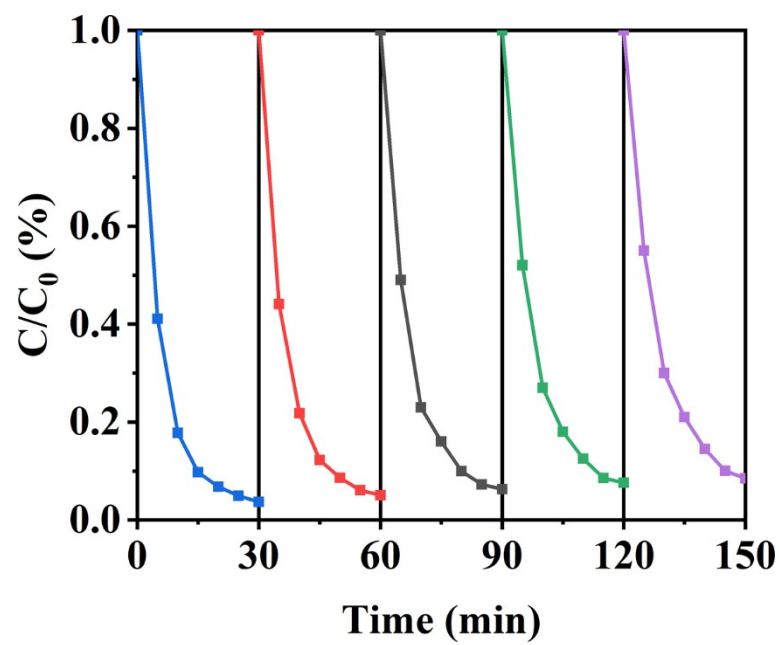


Fig. S12 Cyclic photocatalytic reaction of T101-V_O.

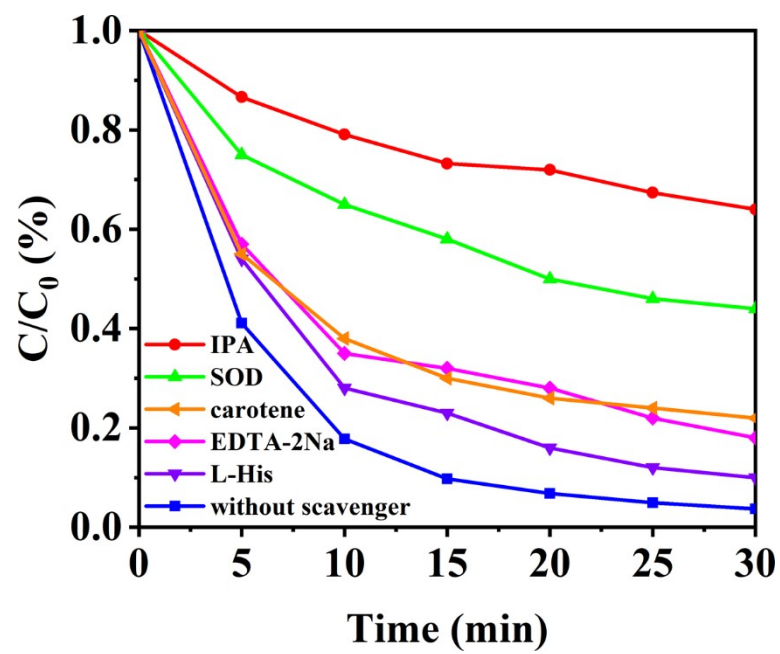


Fig. S13 Photodegradation of RhB by T101-V_O under different conditions.

References

- 1 J. Yu, J. Low, W. Xiao, P. Zhou and M. Jaroniec, *J. Am. Chem. Soc.*, 2014, **136**, 8839-8842.
- 2 L. Liu, Y. Jiang, H. Zhao, J. Chen, J. Cheng, K. Yang and Y. Li, *ACS Catal.*, 2016, **6**, 1097-1108.