

Support Information

1. UV analysis of the samples

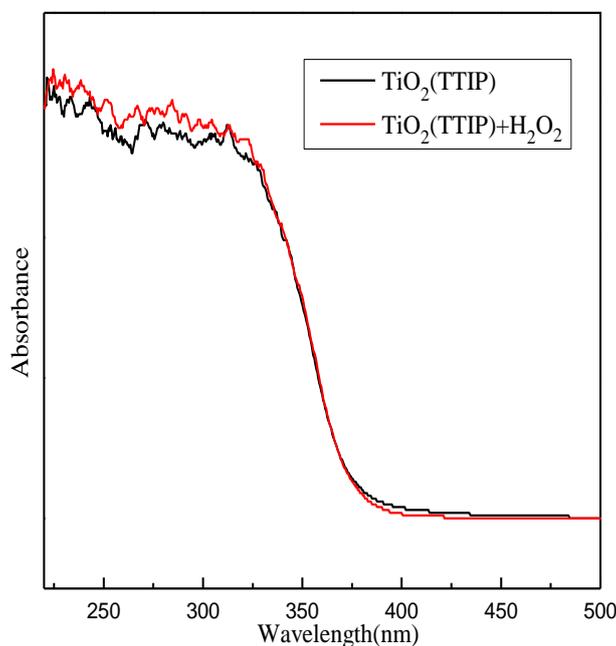


Fig. S1 Diffuse reflectance UV-vis spectra of TiO₂-TTIP before and after treatment with H₂O₂.

2. XPS analysis of the samples

The TiO₂-TBOT samples was prepared and post-treated by the same method as the references reported. The existence of Ti⁴⁺ and Ti³⁺ was proved before and after the treatment with H₂O₂ in TiO₂-TBOT [1, 2, 3]. An obvious peak at 458.7eV and 464.4eV set corresponding to the Ti⁴⁺ state (Ti 2p_{1/2} and 2p_{3/2}) was detected for AT-TBOT in Fig. S2(A) and Fig. S2(B). After the H₂O₂ treatment, The one at 531.8 eV is attributed to Ti³⁺ (Ti³⁺-O) and Ti⁴⁺-OH in Fig. S2(C).

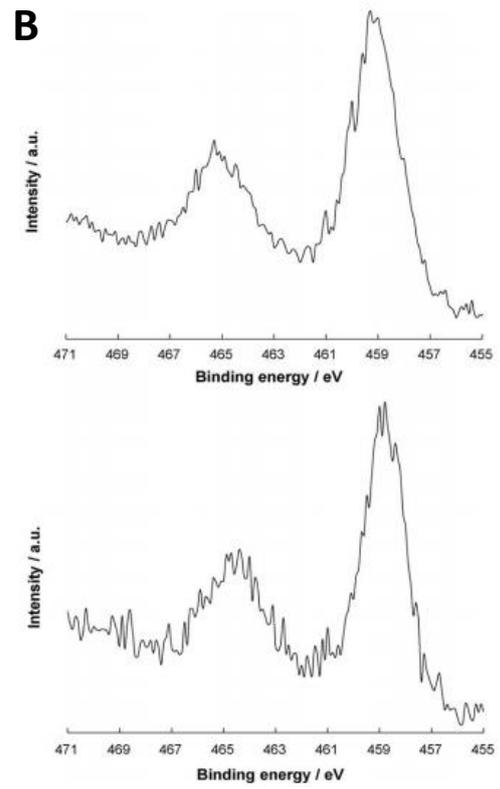
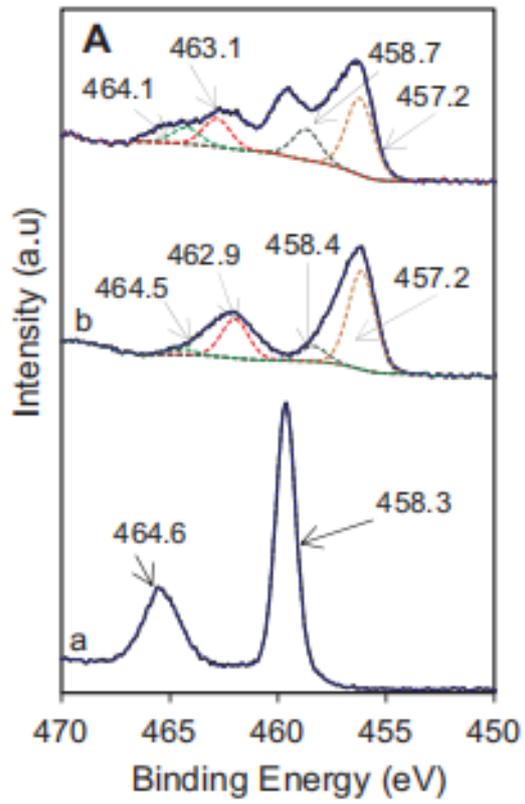


Fig. S2 XPS spectra of (A) Ti 2p and (B) the TiO₂ film [1, 2]

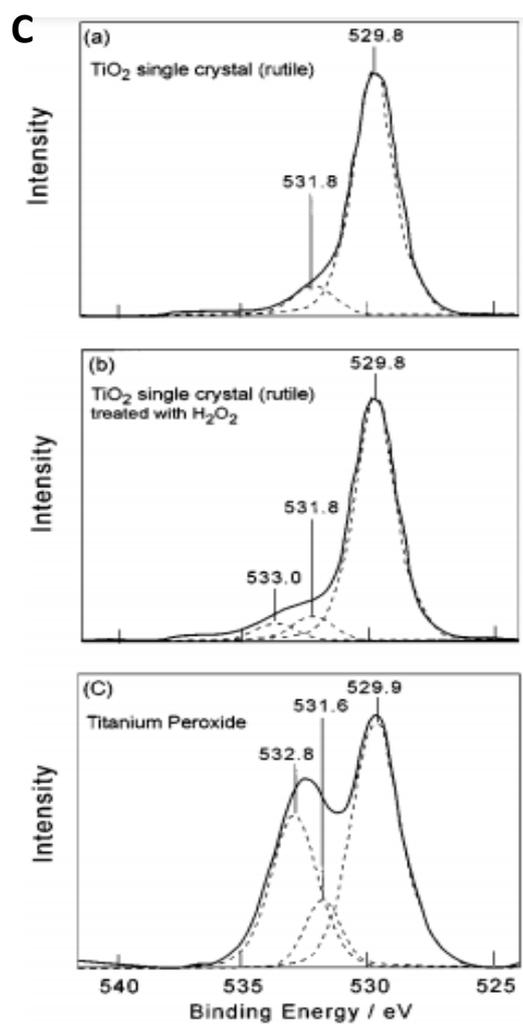


Fig. S2(C) X-ray photoelectron spectra of the O1s band of a $\text{TiO}_2(001)$ single crystal before (a) and after (b) the treatment with H_2O_2 , and that of a Ti-peroxide powder (c) [3]

3. Analysis of masking experiment of hydroxyl radicals

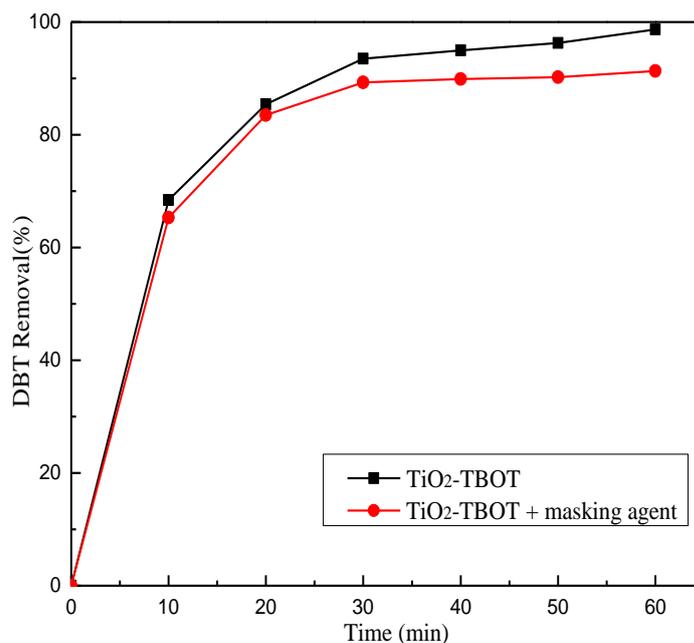


Fig. S3 The impact of masking agent (tert-butyl alcohol) on the removal of DBT

for TiO₂-TBOT. Reaction conditions: m (catalyst) = 0.1 g, T = 60°C,

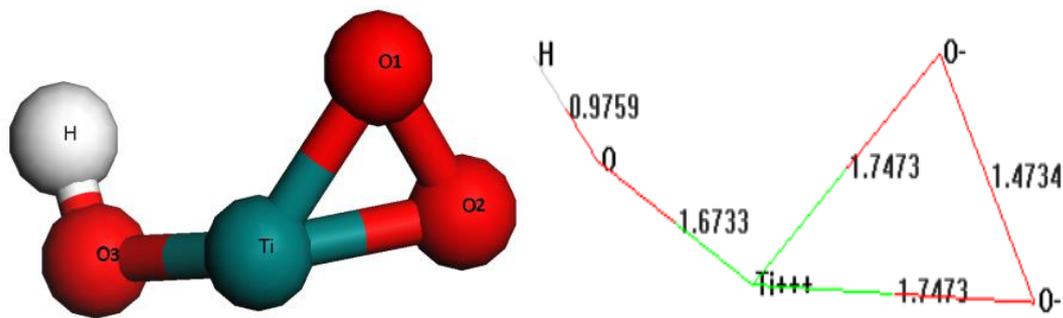
$n(\text{H}_2\text{O}_2)/n(\text{DBT}) = 4$, $v(\text{oil})/v(\text{methanol}) = 1 : 1$, $t = 60$ min.

Tert-butyl alcohol was used as a probe to explore the catalytic mechanism of TiO₂-TBOT in this experiment. Fig. S3 shows that the desulfurization rate does not change obviously after adding appropriate amount of tert-butanol as masking agent, and it stabilizes at about 90% after 20 minutes. This indirectly proves that ·OH does not play a key role in this reaction.

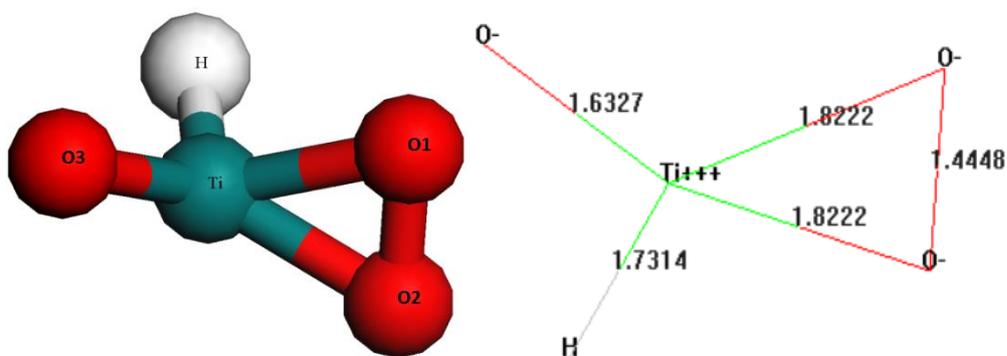
4. Molecular structure modeling

General computational method

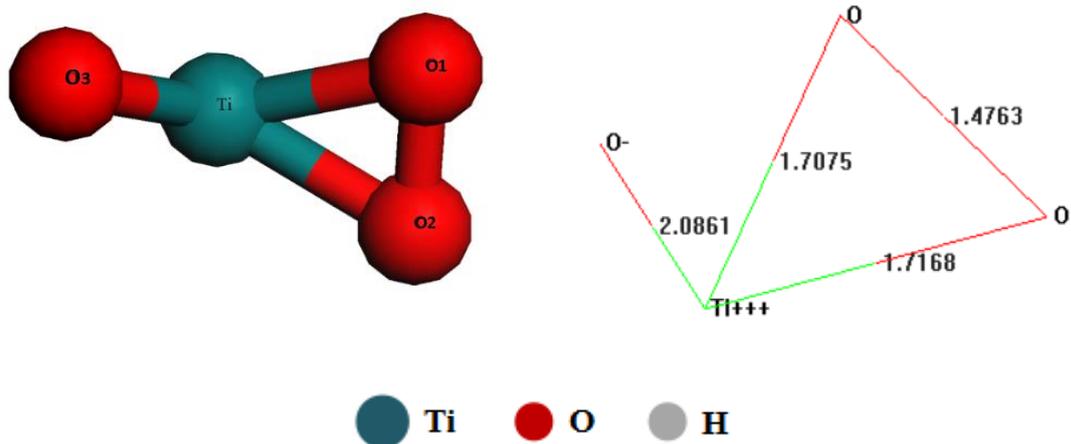
The calculations were performed by HyperChem program. All of the structures of the molecules were optimized until energy minimized through quantum chemistry ab initio method at the ST0-3G level in the software of HyperChem.



Scheme S1(a) Molecular structure modeling of active component



Scheme S1(b) Molecular structure modeling of active component



Scheme S1(c) Molecular structure modeling of active component

Scheme S1(a) and Scheme S1(b) show the bond lengths of the Ti-O with mobilizable proton in active component of two possible configurations. The bond length of Ti-O3 is shorter than the length of Ti-O1 and Ti-O2 in the molecular

structures with a proton. [Scheme S1\(c\)](#) shows the bond length of Ti-O3 is longer than the other Ti-O bond without a proton.

参考文献

1. C. N. Hitam, A. A. Jalil, S. Triwahyono, et al. Fuel, 2018, **216**: 407-417.
2. M. E. Simonsen, Z. Li, G.S. Erik, Appl. Surf. Sci, 2009, **255**(18):8054-8062.
3. T. Ohno, Y. Masaki, S. Hirayama, et al. J. Catal, 2001, **204**(1):163-168.