Supplementary Information

Effects of size on the photocatalytic property of high-index faceted pseudocubic and rhombohedral α-Fe_2O_3 nanocrystals

[a]Ministry Key Laboratory of Oil and Gas Fine Chemicals, College of the Chemistry and Chemical Engineering, Xinjiang University, Urumqi 830046, China.

[b]Guangdong Provincial Key Laboratory of Petrochemcial Pollution Processes and Control, School of E nvironmental Science and Engineering, Guangdong University of Petrochemical Technology, Maomin g, Guangdong 525000, China

[c]The Key Laboratory of Pollution Control and Ecosystem Restoration in Industry Clusters (Ministry of Education), School of Environment and Energy, South China University of Technology, Guangzhou 510006, China.

*Corresponding author:

Email: jerryyang1924@163.com

Quantum yield calculation

$$\Phi = 4\times \frac{\text{initial rate of } O_2 \text{ production (mol s}^{-1})}{\text{photo flux (mol s}^{-1})}$$ (4 photons absorbed per O_2).

Taking the Fe_2O_3-6.0 as an example

Using a wavelength of 420 nm, the intensity of light measured at 100 mW/cm^2, impinging on 7 cm^2 surface area. O_2 released at the 2 min reaction time was used for determining.

Energy of a single photon at 420 nm = h.c/l = $6.626 \times 10^{-34} \times 2.998 \times 10^{8}/ (420 \times 10^{-9}) = 4.730 \times 10^{-19}$ J

Total power absorbed = 7 cm^2 × 100 mW/cm^2 × 2× 60 s = 84 J

Number of O_2 molecules produced = 7.32 µmol × 6.022 × 10^{23} = 4.41× 10^{18}

Quantum Yield O_2 = 4.41 × 10^{18}/(84 J/4.73 × 10^{-19} J) × 400 % = 9.93 %

Turn over Frequency calculation

Taking the Fe_2O_3-6.0 as an example

Moles of Fe = 2×5 mg/159.6882 g mol^{-1} = 6.26 × 10^{-5} mol

The production of O_2 = 7.32 µmol (2 min)

TOF = 7.32 µmol/6.26 × 10^{-5} mol/120 s

TOF = 0.97 × 10^{-3} mol (O_2)/mol (Fe) s

TOF for other catalysts were determined similarly.

The computational process of the valence band and conduction band of α-Fe_2O_3:

$$E_{CB} = X - E_C - \frac{1}{2}E_g$$

$$X = \sqrt[x+y]{X_{Fe}{}^{x} \times X_O{}^{y}}$$
$$= \sqrt[5]{4.06^2 \times 7.54^3}$$
$$= 5.886\ eV$$

Taking the Fe_2O_3-6.0 as an example

E_g=1.964 eV

E_{CB} =5.886 - 4.5 - 0.5×1.964

=0.404 eV

$E_{VB} = E_{CB} + E_g$

=0.404 + 1.964

=2.368 eV