

Preparation and enhanced visible-light photocatalytic H₂-production activity of CdS-sensitized Pt/TiO₂ nanosheets with exposed (001) facets

Lifang Qi^a, Jiaguo Yu^{a,*} and Mietek Jaroniec^{b,*}

^aState Key Laboratory of Advanced Technology for Material Synthesis and Processing, Wuhan University of Technology, Luoshi Road 122#, Wuhan 430070, P. R. China

E-mail: jiaguoyu@yahoo.com

^bDepartment of Chemistry, Kent State University, Kent, Ohio, 44242, USA

E-mail: jaroniec@kent.edu

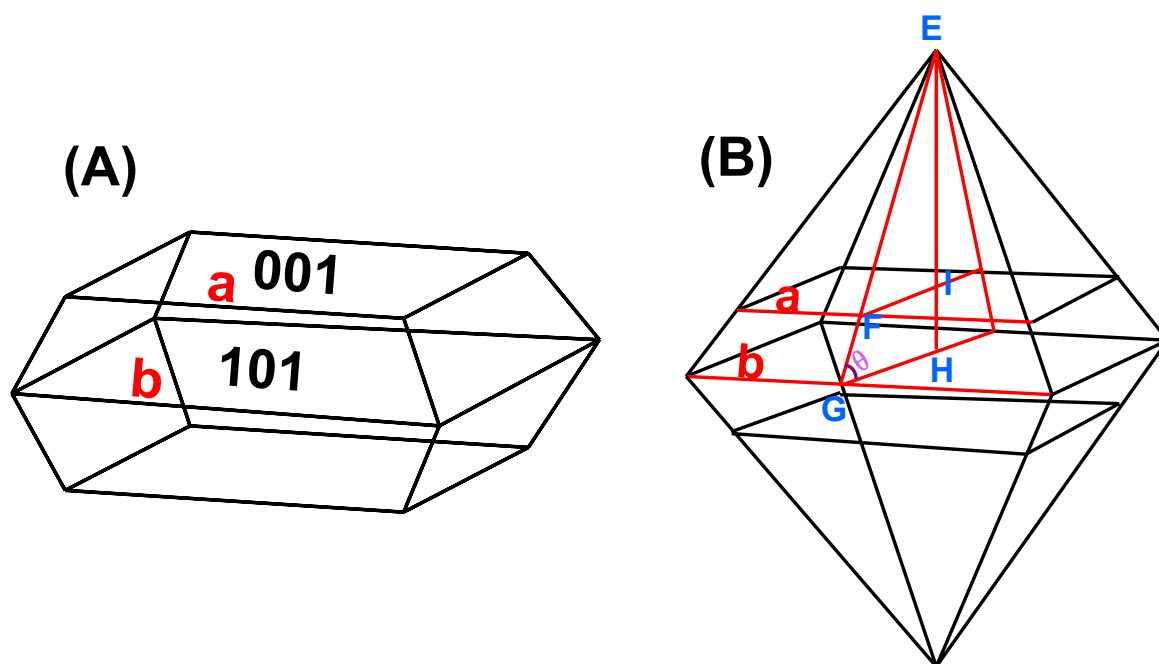


Fig. S1. A) Slab model of anatase TiO₂ single crystal. B) Equilibrium model of anatase TiO₂ single crystal.

C) Calculation of percentage of {001} facets is as follows:

$$S_{001} = 2a^2$$

$$S_{101} = 8(\frac{1}{2}EG \times b - \frac{1}{2}EF \times a)$$

$$\begin{aligned} S_{001} \% &= \frac{S_{001}}{S_{001} + S_{101}} \\ &= \frac{2a^2}{2a^2 + 8(\frac{1}{2}EG \times b - \frac{1}{2}EF \times a)} \\ &= \frac{a^2}{a^2 + 4(\frac{1}{2} \times \frac{\frac{1}{2}b}{\cos \theta} \times b - \frac{1}{2} \times \frac{\frac{1}{2}a}{\cos \theta} \times a)} \\ &= \frac{a^2}{a^2 + \frac{b^2 - a^2}{\cos \theta}} = \frac{1}{1 + \frac{\frac{b^2}{a^2} - 1}{\cos \theta}} = \frac{\cos \theta}{\cos \theta + \frac{b^2}{a^2} - 1} = \frac{\cos \theta}{\cos \theta + (\frac{a}{b})^{-2} - 1} \\ &= \frac{\cos 68.3^\circ}{\cos 68.3^\circ + (\frac{75.5}{80})^{-2} - 1} = 75.0\% \end{aligned}$$

Here θ is the theoretical value for the angle between the [001] and [101] facets of anatase. As indicated in the slab model, two independent parameters b and a denote lengths of the side of the bipyramid and the side of the square {001} ‘truncation’ facets, respectively. The ratio of highly reactive {001} facets to total surface area can thus be described by the value of S_{001}/S or a/b (where $0 \leq a/b \leq 1$). a/b is the degree of truncation).

References

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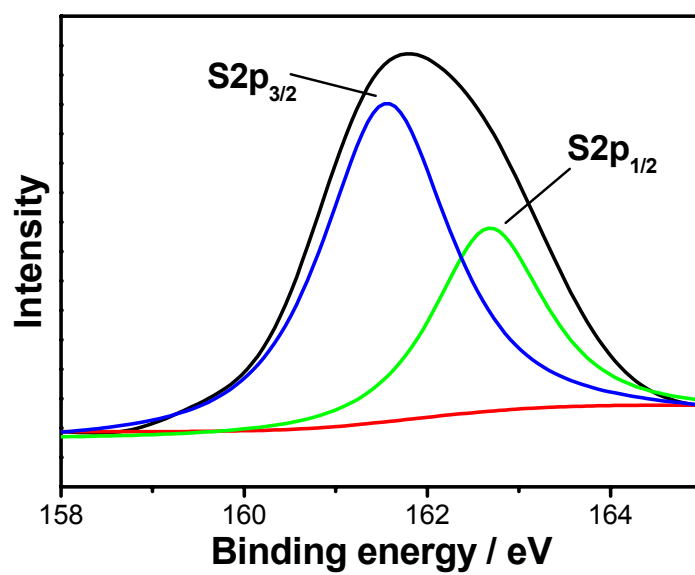


Fig. S2. High-resolution XPS spectrum of S2p for sample HQ1.