Crystal-Plane-Dependent Guaiacol Hydrodeoxygenation Performance of Au on Anatase TiO_2

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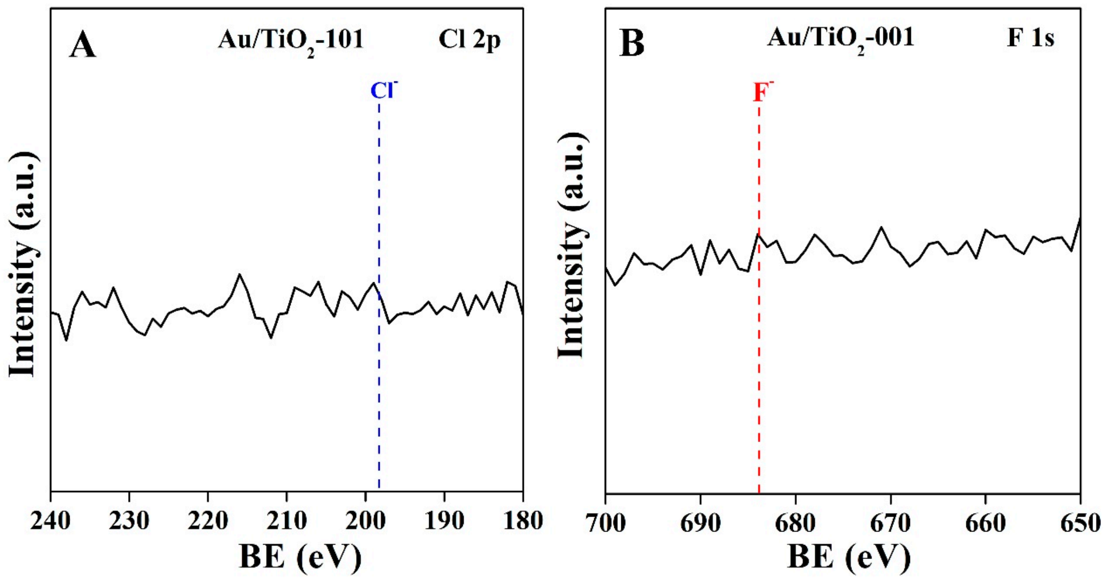


Figure S1. XPS spectrum of Cl 2p and F 1s in the Au/TiO_2-101(**A**) and Au/TiO_2-001(**B**)

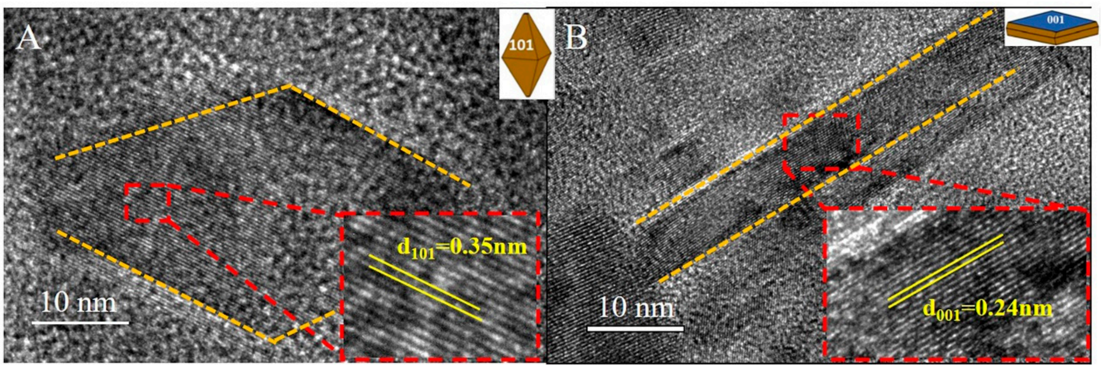


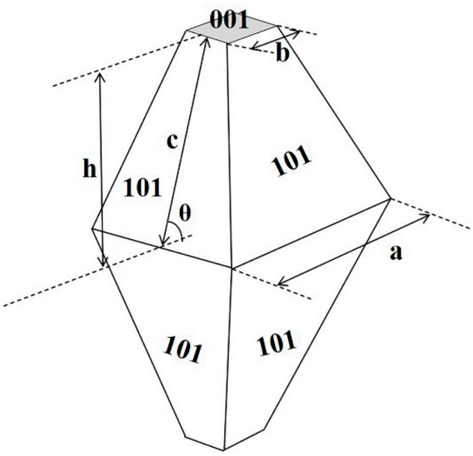
Figure S2. HRTEM images of TiO_2-101(**A**), TiO_2-001(**B**)

Table S1. The percentages of different crystal planes in the as-prepared TiO_2 nanocrystals were based on geometric calculation.

Samples	101	001
TiO_2-101	95.9 %	4.1 %
TiO_2-001	15.8 %	84.2 %

Based on the statistical analysis of TEM and HRTEM images of TiO_2-101 and TiO_2-001 and assuming the ideal crystal models expected from the Wulff Construction, we calculated the percentages of different facet orientations for the different types of TiO_2 nanocrystals.

(1). TiO_2-101 nanocrystals



a=13.1 ± 0.18 nm

b=4.1 ± 0.16 nm

h=16.4 ± 0.35 nm

θ=68.3°

Figure S3. Geometric model of TiO_2-101 nanocrystals.

There are two kinds of crystal planes exposed in TiO_2-101 sample: 101 and 001. We can figure out the percentages of 101 and 100 in TiO_2-101 nanocrystals as follows:

$$c = \frac{h}{\sin\theta}$$

$$S_{101} = \frac{1}{2}(a+b)\mathrm{c}$$

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

$$P_{101} = \frac{S_{101}\times 8}{S_{101}\times 8 + S_{001}\times 2}$$

$$P_{001} = \frac{S_{001}\times 2}{S_{101}\times 8 + S_{001}\times 2}$$

(2). TiO_2-001 nanocrystals

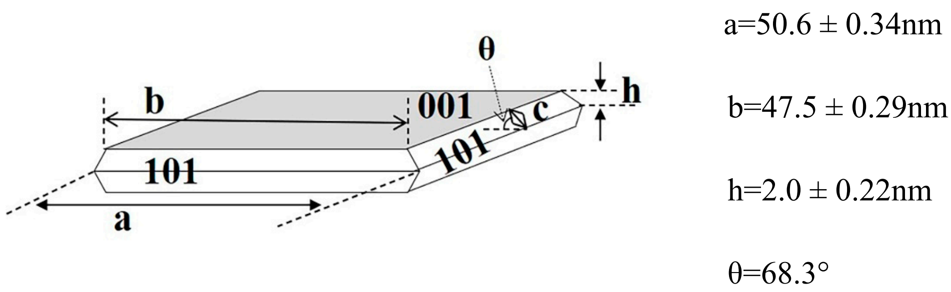


Figure S4. Geometric model of TiO_2-001 nanocrystals.

There are two kinds of crystal planes exposed in TiO_2-001 sample: 101 and 001. We can figure out the percentages of 101 and 100 in TiO_2-001 nanocrystals as follows:

$$c = \frac{h}{\sin\theta}$$

$$S_{101} = \frac{1}{2}(a+b)\mathrm{c}$$

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

$$P_{101} = \frac{S_{101}\times 8}{S_{101}\times 8 + S_{001}\times 2}$$

$$P_{001} = \frac{S_{001}\times 2}{S_{101}\times 8 + S_{001}\times 2}$$

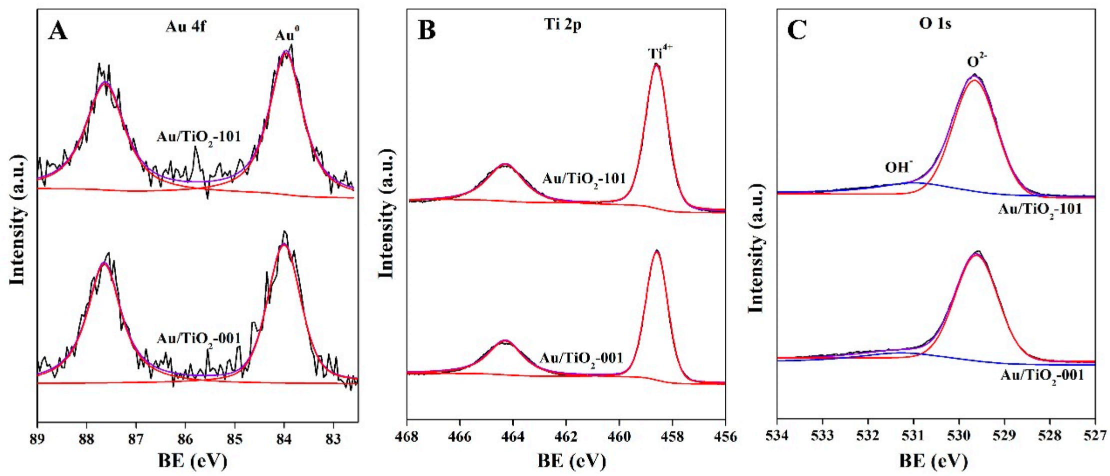


Figure S5. XPS spectrum of Au 4f (**A**), Ti 2p (**B**) and O 1s (**C**) in Au/TiO_2 catalysts before *in-situ* reduction

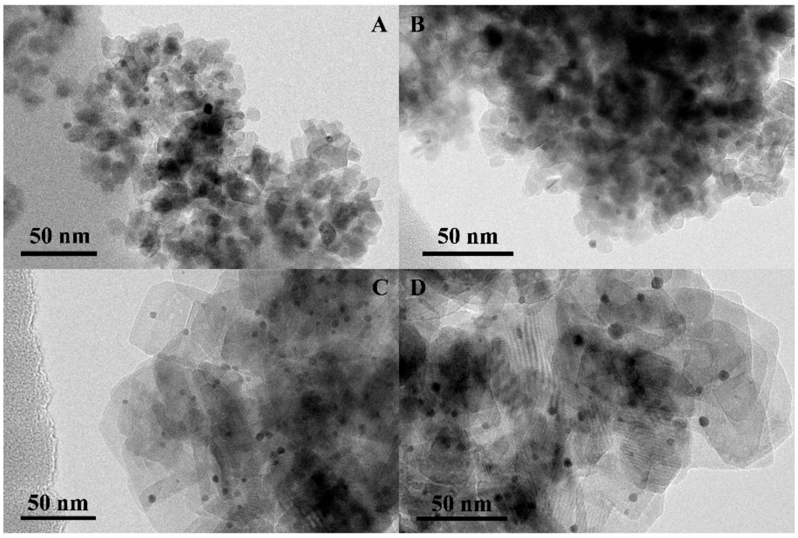


Figure S6. TEM images of Au/TiO_2 catalyst before and after pre-treatment. Au/TiO_2-101-before (**A**), Au/TiO_2-101-after (**B**), Au/TiO_2-001-before (**C**) and Au/TiO_2-001-after (**D**)