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锐钛矿型 TiO_2 担载的 Pd 催化剂用于乙炔选择加氢的催化性能及其表征

高晓平 [1,2] 郭章龙 [1,2] 周亚男 [1,2] 敬方梨 [1] 储伟 [1,2,*]

([1] 四川大学化学工程学院，成都 610065；[2] 四川大学新能源与低碳技术研究院，成都 610207)

Catalytic Performance and Characterization of Anatase TiO_2 Supported Pd Catalysts for the Selective Hydrogenation of Acetylene

GAO Xiao-Ping[1,2] GUO Zhang-Long[1,2] ZHOU Ya-Nan[1,2] JING Fang-Li[1]

CHU Wei[1,2,*]

([1]*School of Chemical Engineering, Sichuan University, Chengdu 610065, P. R. China*; [2]*Institute of New Energy and Low-Carbon Technology, Sichuan University, Chengdu 610207, P. R. China*)

[*]Corresponding author. Email: chuwei1965@scu.edu.cn; Tel: +86-28-85403836.

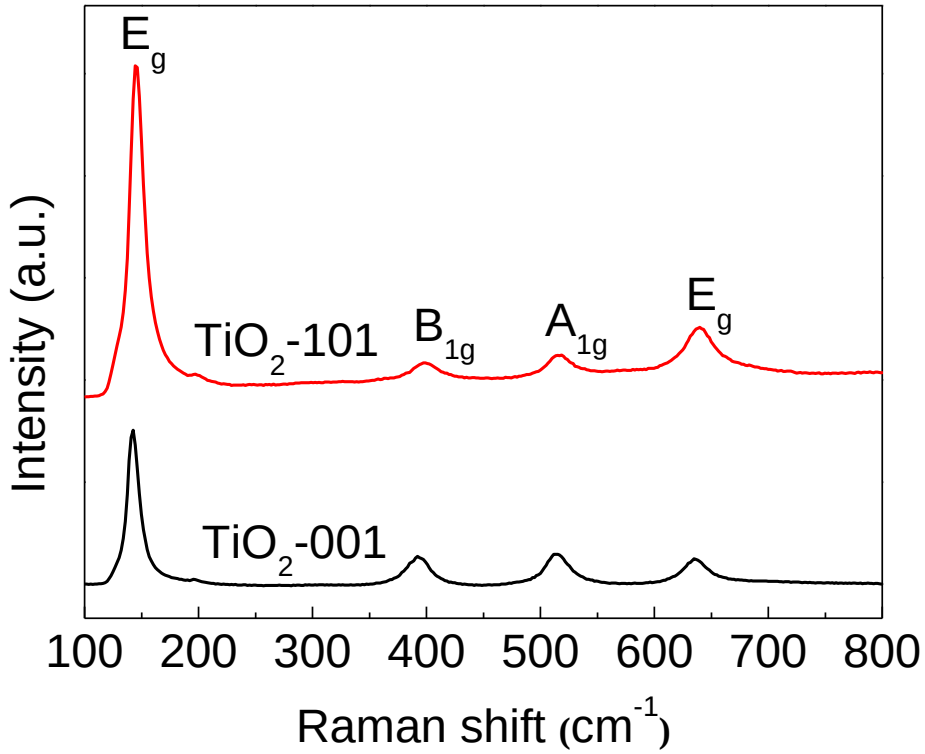


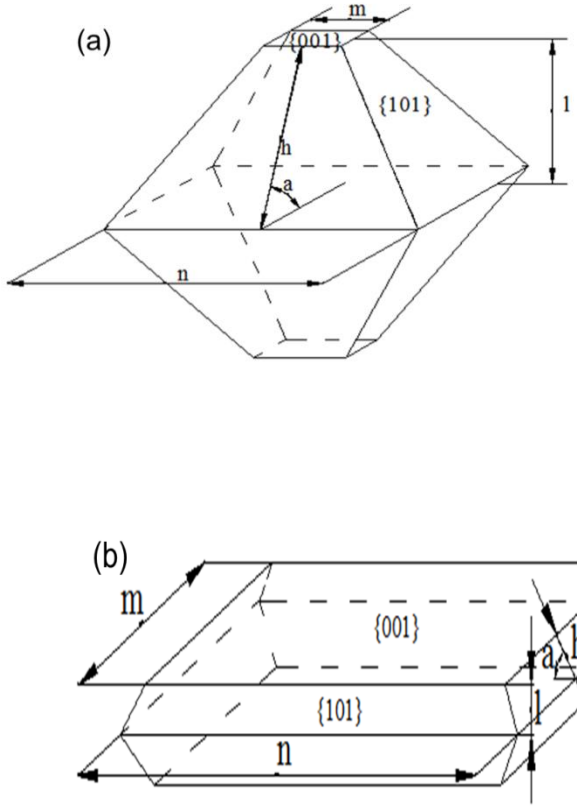
Fig.S1 Raman spectra of TiO_2 nanoparticles

Fig.S1 displayed Raman spectra of TiO_2 nanoparticles. Both samples were of the similar peaks appearing at 144, 394, 514, 636 cm^{-1}, but their intensities varied significantly. It is indicated the typical anatase TiO_2 phase and was also in agreement with the XRD results. E_g peaks at 144 and 636 cm^{-1} were ascribed to the symmetric stretching vibration of O-Ti-O; while the B1g peak at 394 cm^{-1} and A_{1g} peak at 514 cm^{-1} represented the symmetric and anti-symmetric bending vibrations of O-Ti-O, respectively. However, the intensity of the E_g peak in the TiO_2-001 sample weakened significantly, mainly because of the selective exposure of the {001} facets. The {001} facet is terminated with unsaturated five-fold Ti atoms (Ti_{5C}) and two-fold O atoms (O_{2C}) [1], which weakened the symmetric stretching vibration of O-Ti-O. This result further confirms the preferential exposure of the {001} facets on the TiO_2 nanosheets.

According to Wulff Construction, the schematic ideal crystal models of TiO_2-101 and TiO_2-101 were shown in Fig.S2(a) and Fig.S2(b), respectively. The proportion of each could be calculated by the following formulae:

$$P_{001}=\frac{S_{001}\times 2}{S_{001}\times 2+S_{101}\times 8}\times 100\% \quad \text{and} \quad P_{101}=\frac{S_{101}\times 8}{S_{001}\times 2+S_{101}\times 8}\times 100\%$$

In our cases, the geometrical parameters of the two TiO_2 nanocrystals could be easily obtained from the TEM results, which provide the opportunity to do such a calculation. As a results, the percentages of {101} facets and {001} facets in TiO_2-101 nanospindles are 89% and 11%, while those in TiO_2-001 nanosheet are 23% and 77%, respectively.



m = 7.74 nm

n = 15.7 nm

l = 10 nm

a = 68.3°

$\boldsymbol{h} = \frac{l}{\sin a}$

$S_{101} = \frac{1}{2}(\boldsymbol{m}+\boldsymbol{n})\times \boldsymbol{h}$

$S_{001} = \boldsymbol{m}^2$

m = 38 nm

n = 40 nm

l = 2.5 nm

a = 68.3°

$\boldsymbol{h} = \frac{l}{\sin a}$

$S_{001} = \boldsymbol{m}^2$

$S_{101} = \frac{1}{2}(\boldsymbol{m}+\boldsymbol{n}) \times \boldsymbol{h}$

Fig.S2 Ideal crystal models of (a) TiO_2-101 and (b) TiO_2-001

References about the Wullf construction and related calculations are from Ref.2-4.

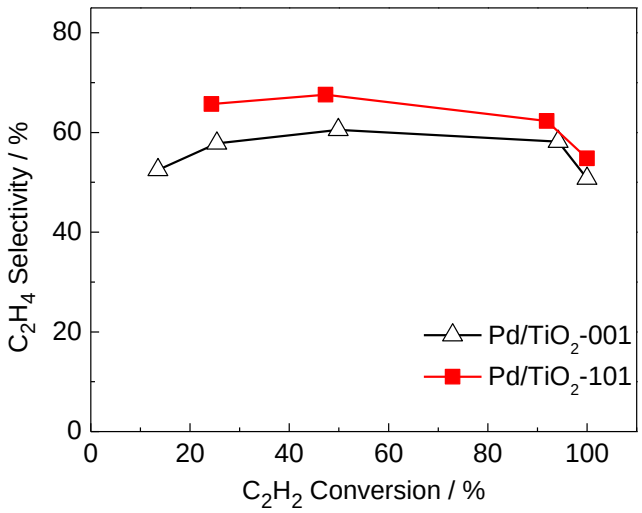


Fig.S3 Ethylene selectivity *versus* acetylene conversion over Pd/TiO_2-001 and Pd/TiO_2-101 catalysts at a total flow rate of 50 mL·min^{-1} with varying reaction temperatures from 40 to 80 ℃

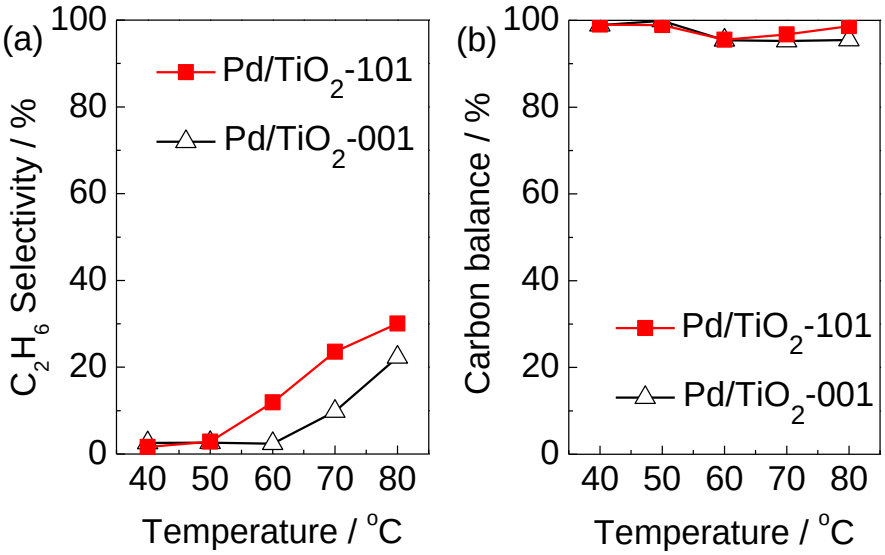


Fig.S4 Selectivity to ethane (a) and the carbon balance (b) *versus* temperature over Pd/TiO_2-001 and Pd/TiO_2-101 catalysts at a total flow rate of 50 mL·min^{-1} with varying reaction temperatures from 40 to 80 ℃

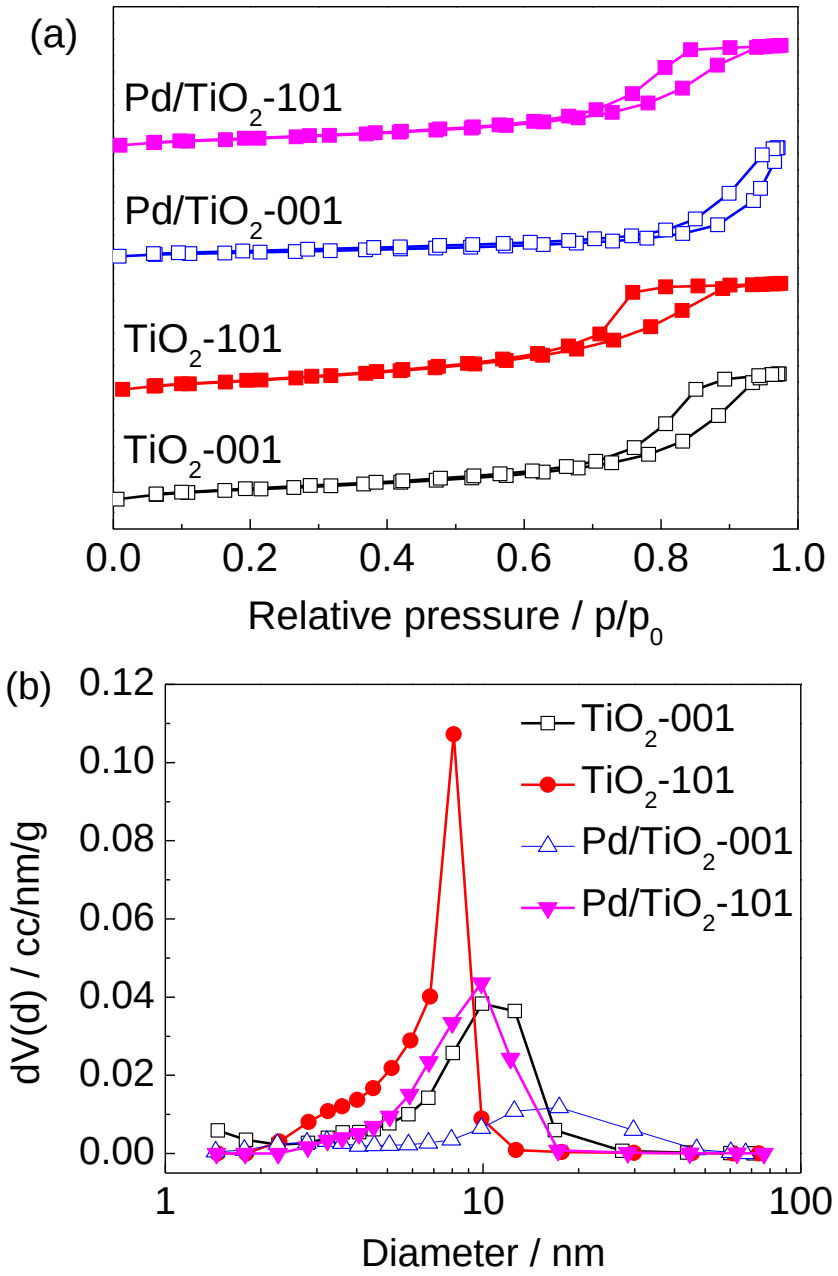


Fig.S5 (a) Nitrogen adsorption-desorption isotherms, and (b) BJH pore-size distributions

Table S1 Summary of physical properties of TiO_2 nanoparticles and Pd/TiO_2 catalysts

Sample	Surface area/($m^2 \cdot g^{-1}$)	Pore volume/($cm^3 \cdot g^{-1}$)	Pore diameter/nm
TiO_2-001	93	0.3127	13.38
1%Pd/TiO_2-001	51	0.2698	21.34
TiO_2-101	124	0.2757	8.887
1%Pd/TiO_2-101	89	0.2590	11.59

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