

## Supporting Information of

# Coordinately unsaturated O<sub>2c</sub>–Ti<sub>5c</sub>–O<sub>2c</sub> sites promote the reactivity of Pt/TiO<sub>2</sub> catalysts in the solvent-free oxidation of octanol

*Pengfei Yang<sup>1</sup>, Mark Douthwaite<sup>2</sup>, Jiahao Pan<sup>1</sup>, Lirong Zheng<sup>3</sup>, Song Hong<sup>1</sup>, David J. Morgan<sup>2</sup>, Mingyu Gao<sup>1</sup>, Dianqing Li<sup>1</sup>, Junting Feng<sup>1\*</sup>, and Graham J. Hutchings<sup>2\*</sup>*

<sup>1</sup> State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical Technology, People's Republic of China

<sup>2</sup> Max Planck- Cardiff Centre on the Fundamentals of Heterogeneous Catalysis FUNCAT, Cardiff Catalysis Institute, School of Chemistry, Cardiff University, Main Building, Park Place, Cardiff, CF10 3AT (UK)

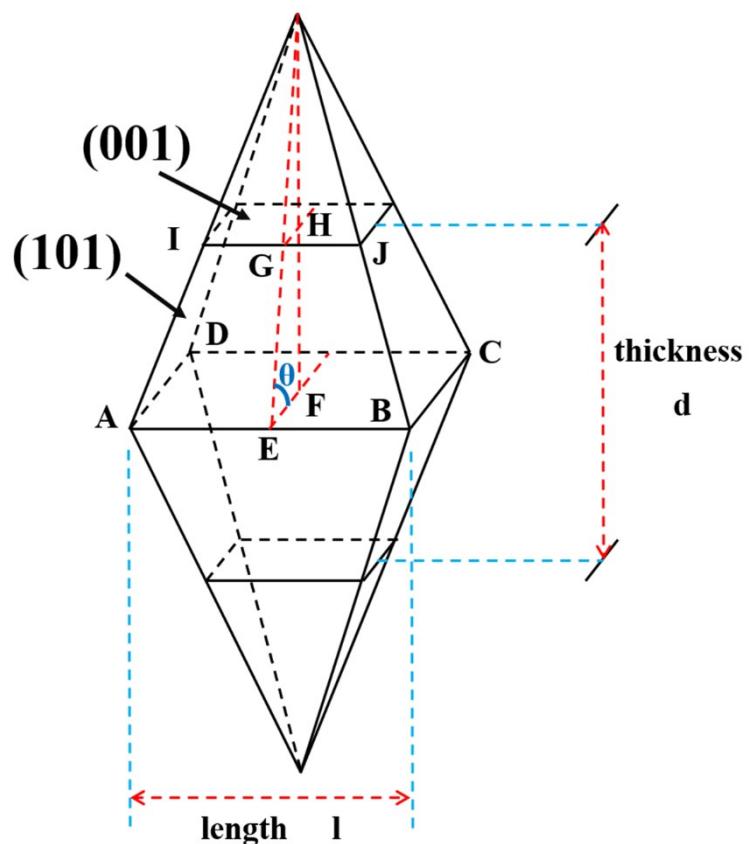
<sup>3</sup> Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, People's Republic of China

\* Corresponding author

Address: Box 98, 15 Bei San Huan East Road, Beijing 100029, China

Tel: +86 10 64436992      Fax: +86 10 64436992

E-mail address: [fengjt@mail.buct.edu.cn](mailto:fengjt@mail.buct.edu.cn) (Junting Feng); [Hutch@cardiff.ac.uk](mailto:Hutch@cardiff.ac.uk) (Graham Hutchings)



**Figure S1** A model of anatase  $\text{TiO}_2$  single crystal for calculation of geometrical characteristics.

Table S1 The properties of synthesized  $\text{TiO}_2$  with different facets exposed and the series Pt/ $\text{TiO}_2$  catalysts

	BET surface ( $\text{m}^2/\text{g}$ )	Pt loading (wt.%)
TiO <sub>2</sub> -101	52.0	-
TiO <sub>2</sub> -001	21.8	-
Pt/TiO <sub>2</sub> -101-Air	53.1	0.96
Pt/TiO <sub>2</sub> -001-Air	26.6	0.99
Pt/TiO <sub>2</sub> -101-H <sub>2</sub>	50.1	1.02
Pt/TiO <sub>2</sub> -001-H <sub>2</sub>	24.8	1.01

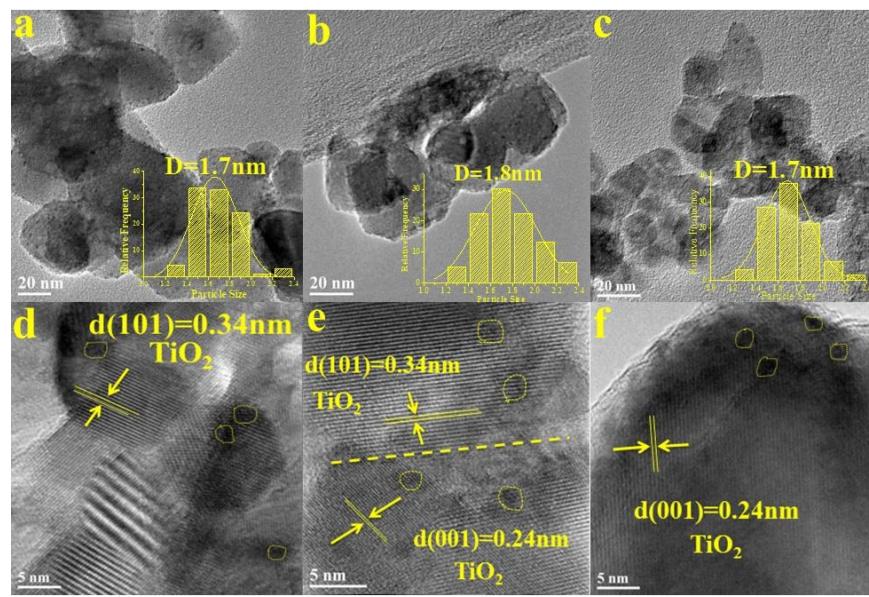


Figure S2 HRTEM images of Pt/TiO<sub>2</sub>-101-Air-500°C (a and d), Pt/TiO<sub>2</sub>-101-001-Air-500°C (b and e) and Pt/TiO<sub>2</sub>-001-Air-500°C(c and f)

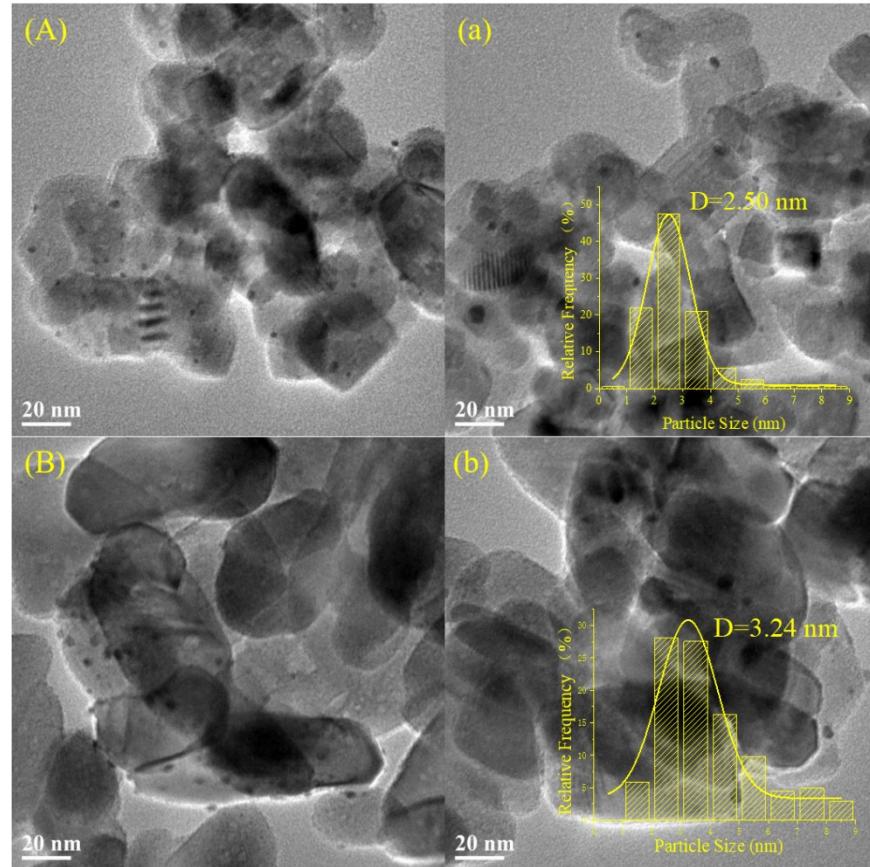


Figure S3 HRTEM images of Pt/TiO<sub>2</sub>-101-H<sub>2</sub> (A and a) and Pt/TiO<sub>2</sub>-001-H<sub>2</sub> (B and b)

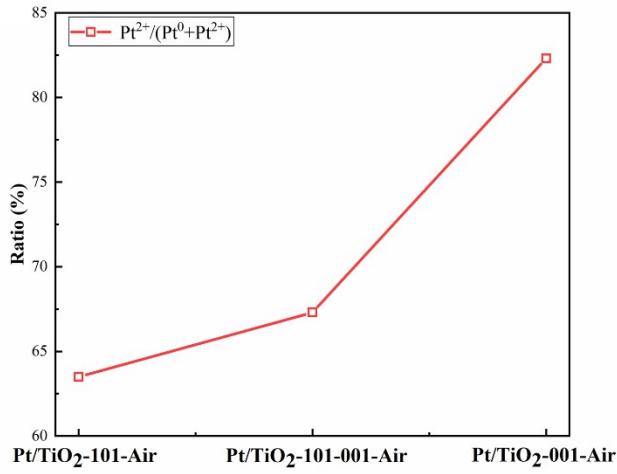


Figure S4 The ratio of  $\text{Pt}^{2+}/(\text{Pt}^{2+}+\text{Pt}^0)$  over the calcined  $\text{Pt}/\text{TiO}_2$  with different facets exposed.

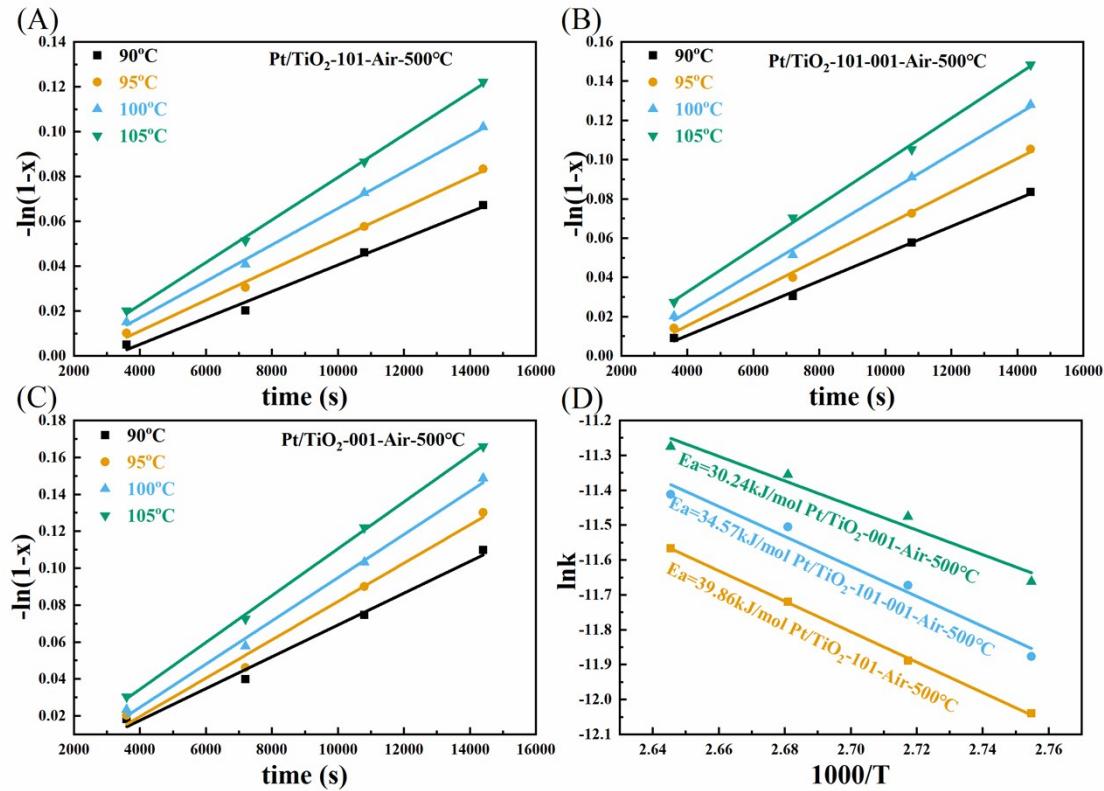


Figure S5 Time–conversion plots at various temperatures for  $\text{Pt}/\text{TiO}_2$ -101-Air (A),  $\text{Pt}/\text{TiO}_2$ -101-001-Air (B), and  $\text{Pt}/\text{TiO}_2$ -001-Air (C) and Arrhenius plots (D) for n-octanol oxidation.

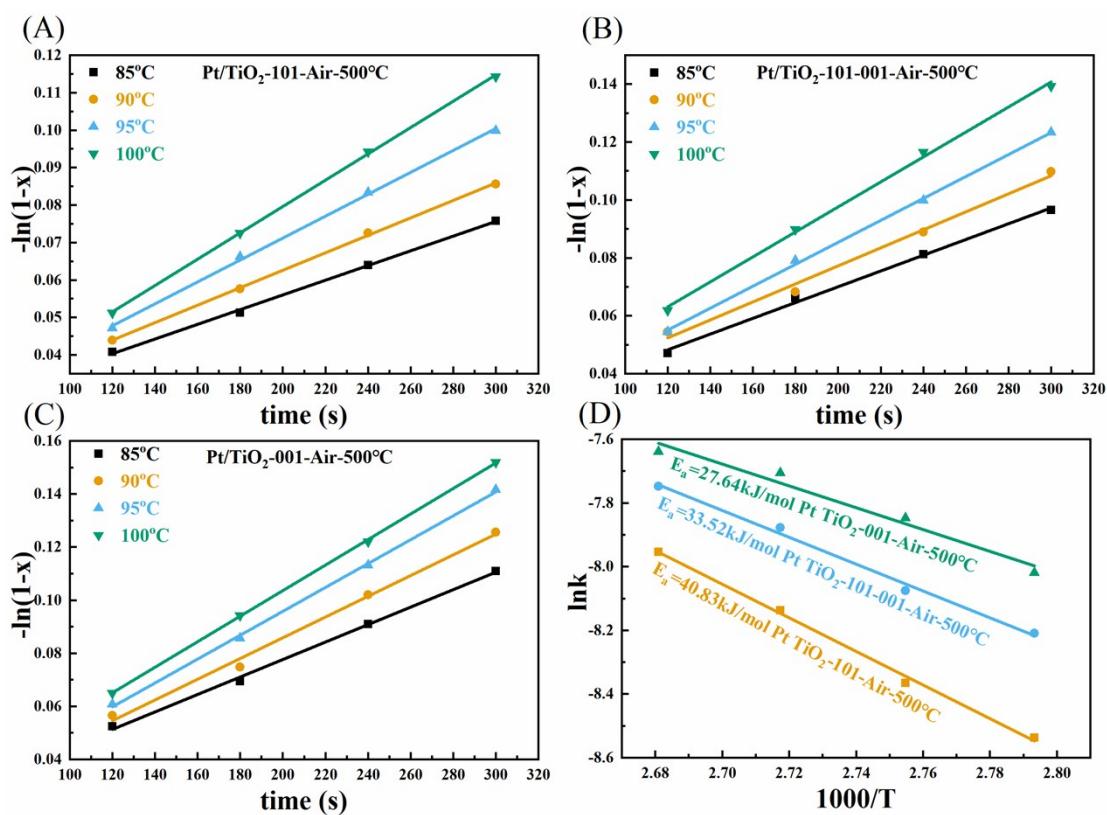


Figure S6 Time–conversion plots at various temperatures for Pt/TiO<sub>2</sub>-101-Air (A), Pt/TiO<sub>2</sub>-101-001-Air (B), and Pt/TiO<sub>2</sub>-001-Air (C) and Arrhenius plots (D) for octanal oxidation.