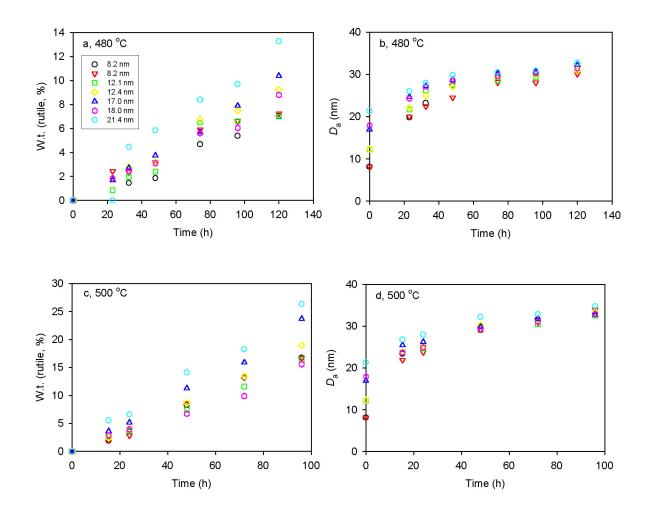
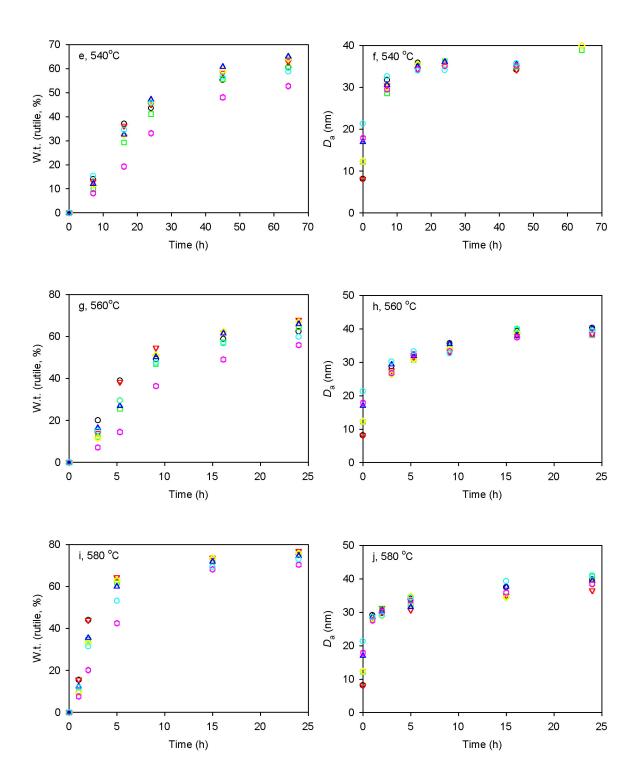
## **Supporting Information For**

# Size-dependence of the kinetic rate constant for phase transformation in **TiO<sub>2</sub>** nanoparticles

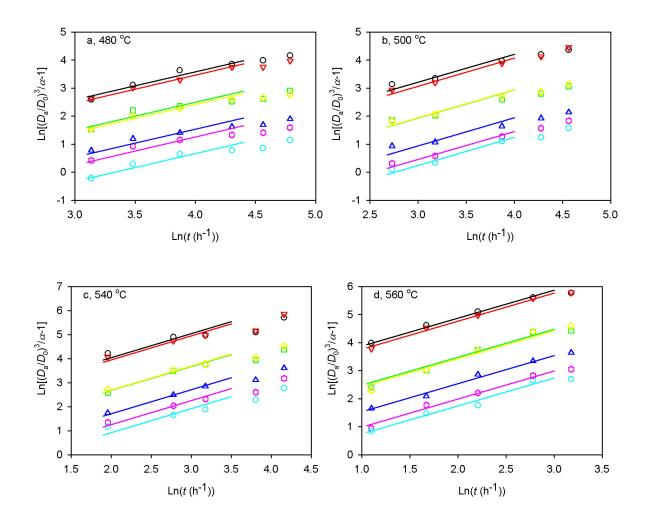
Hengzhong Zhang, Jillian F. Banfield



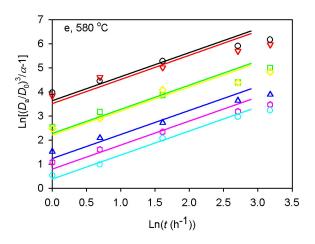
#### 1. Experimental data (480 – 580 °C)



**Figure S1.** Kinetic data for phase transformation of nanocrystalline anatase with various initial particle sizes. Weight percentages of rutile and average particle sizes of anatase for anatase samples heated at 480 °C ( $\mathbf{a}$ ,  $\mathbf{b}$ ), 500 °C ( $\mathbf{c}$ ,  $\mathbf{d}$ ), 540 °C ( $\mathbf{e}$ ,  $\mathbf{f}$ ), 560 °C ( $\mathbf{g}$ ,  $\mathbf{h}$ ), and 580 °C ( $\mathbf{i}$ ,  $\mathbf{j}$ ). Initial particle sizes of anatase (~ 8-21 nm) are indicated in ( $\mathbf{a}$ ). The dispersion in the results as a function of average particle size arises because the phase transformation and crystal growth kinetics depend not just on the average particle size but also on the particle size distribution and the aggregation state (see text).

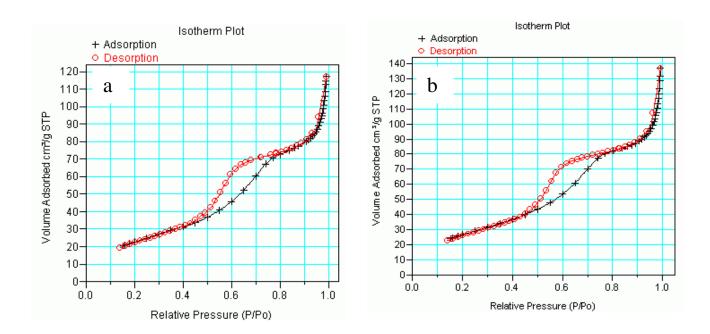


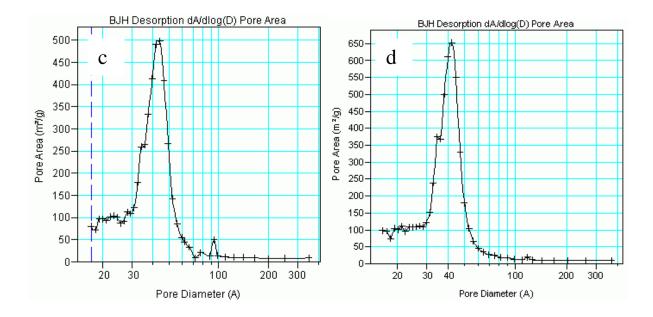
#### 2. Kinetic plots (480 – 580 °C)



**Figure S2.** Kinetic plots (eq1b) for phase transformation of nanocrystalline anatase with various initial sizes. (**a**) 480 °C, (**b**) 500 °C, (**c**) 540 °C, (**d**) 560 °C and (**e**) 580 °C. Lines are from linear least square regressions. This figure adopts the same keys as in Figure **S1a** to indicate the initial particle sizes of anatase.

### 3. Adsorption /desorption isotherms for anatase samples





**Figure S3.** Adsorption/desorption isotherms of nitrogen gas at 77 K on two anatase samples and the pore size distributions in the samples. (**a**) isotherms for 12.4 nm anatase (BET surface area  $86.2 \pm 1.2 \text{ m}^2/\text{g}$ ), (**b**) isotherms for 12.1 nm anatase (BET surface area  $97.0 \pm 1.3 \text{ m}^2/\text{g}$ ), (**c**) pore size distribution on 12.4 nm anatase (cumulative pore area  $119.2 \text{ m}^2/\text{g}$ ), and (**d**) pore size distribution on 12.1 nm anatase (cumulative pore area  $137.8 \text{ m}^2/\text{g}$ ). These results indicate that the 12.4 nm anatase sample has a denser aggregation state than the 12.1 nm anatase sample.

	Average anatase	Specific surface area	Cumulative pore area
Sample #	particle size (nm)	$(m^2/g)$	$(m^{2}/g)$
1	8.2	$162.7 \pm 0.8$	217.4
2	8.2	$150.6 \pm 1.4$	205.0
3	12.1	97.0±1.3	137.8
4	12.4	86.2 ± 1.2	119.2
5	17.0	$45.9 \pm 0.8$	72.0
6	18.0	59.4 ± 0.9	83.6
7	21.4	31.1 ± 0.7	43.3

**Table S1.** Specific surface areas and cumulative pore areas of anatase samples.