

# Supporting Information

## Synthesis of Dodecylphosphonic Acid

15.6 mL (64 mmol) of 1-bromododecane and 12.4 mL (74 mmol) of triethylphosphite were stirred for 3.5 h under refluxing conditions. The lower boiling products were removed by heating at 100 °C under ambient pressure conditions. The excess of triethyl phosphate was removed by distillation under reduced pressure. 13.1 g (42 mmol, 66% yield) of the intermediate product were obtained as a colorless liquid.

Spectroscopic Data of Intermediate-Product:

$^1\text{H}$  NMR( $\text{CDCl}_3$ ,  $\delta$ , ppm): 0.85 (t, 3H,  $\text{CH}_2\text{-CH}_3$ ); 1.22–1.33 (m, 24H,  $-\text{CH}_2-$ ,  $\text{CH}_3\text{-CH}_2\text{-O}$ ); 1.50–1.77 (m, 4H,  $\text{CH}_2\text{-CH}_2\text{-P}$ ); 4.07 (m, 4H,  $\text{CH}_3\text{-CH}_2\text{-O}$ ).

To 13.1 g (42 mmol) of the intermediate product (dodecylphosphonic acid, diethylester) 70 mL of concentrated HCl were added and the reaction mixture was heated to reflux for 22 h. The solvent and volatile byproducts were removed in vacuo. The crude product was washed with acetonitrile several times and dried under reduced pressure. After recrystallisation from n-hexane 9.5 g (90%) of colorless crystals were obtained.

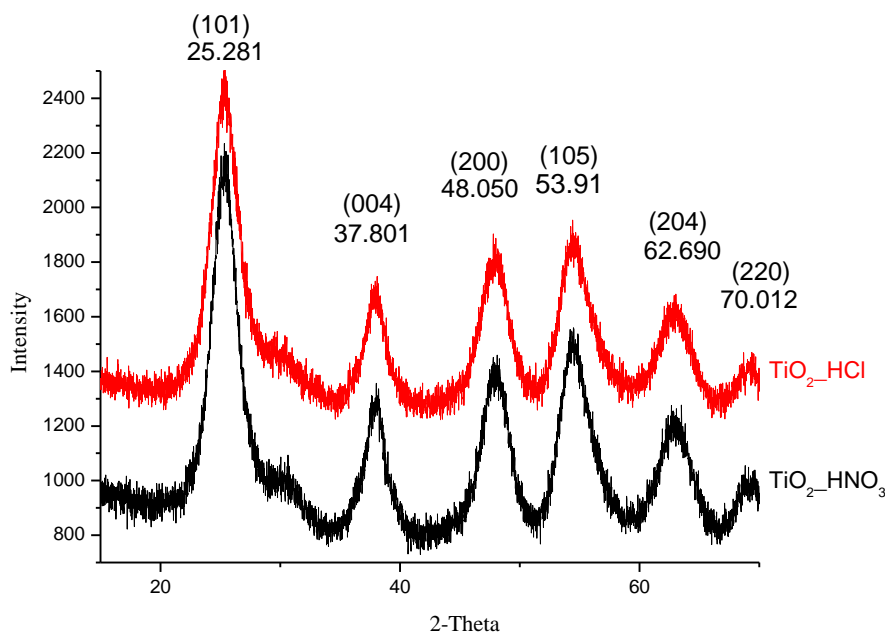
Spectroscopic data for the product:

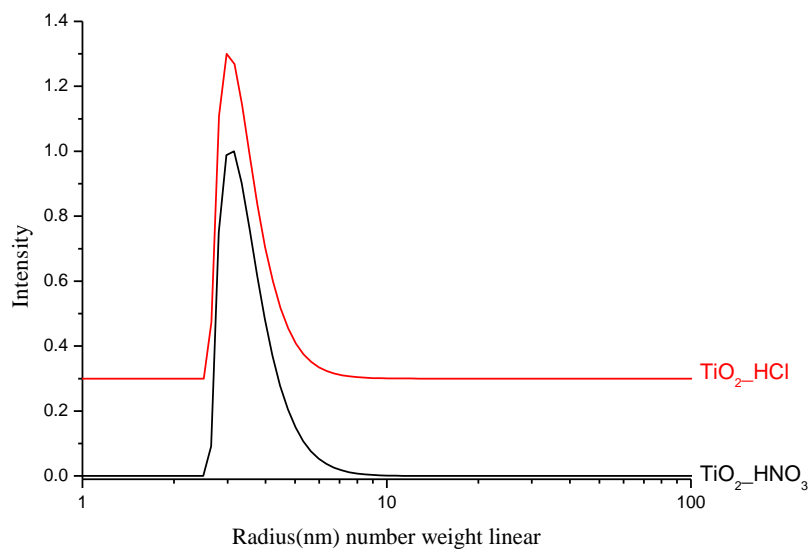
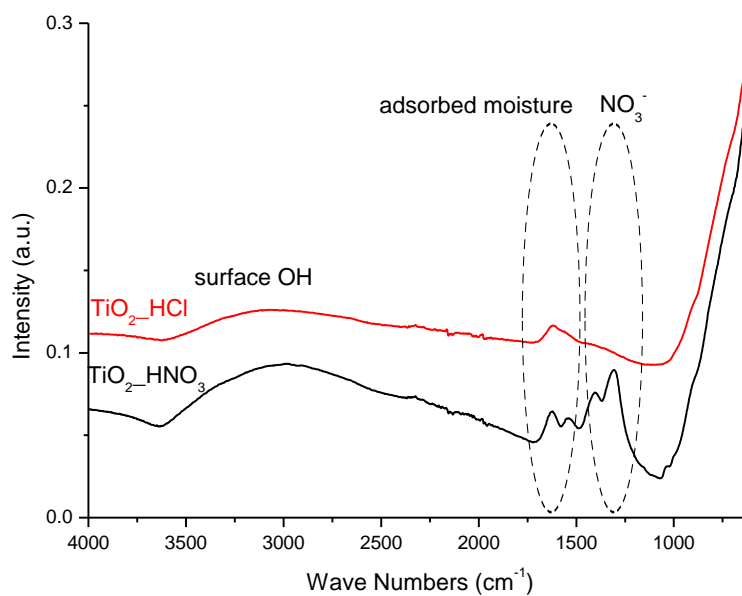
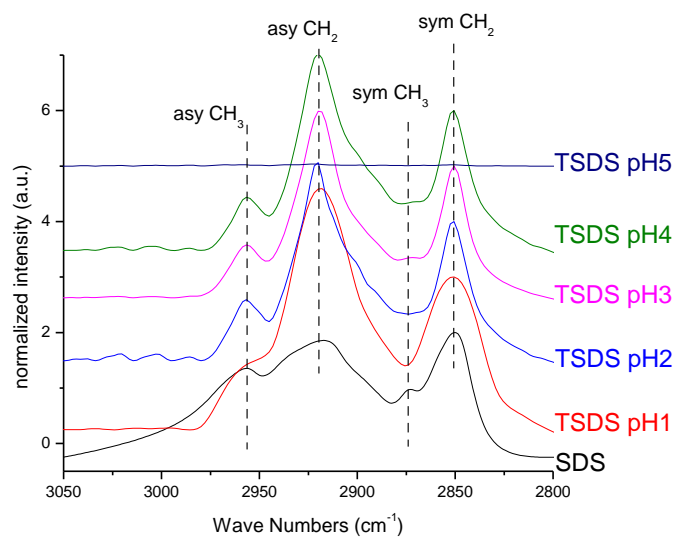
$^1\text{H}$  NMR ( $\text{CDCl}_3$ ,  $\delta$ , ppm): 0.86 (t, 3H,  $\text{CH}_3$ ); 1.20–1.43 (m, 18H,  $-\text{CH}_2-$ ); 1.55–1.82 (m, 4H,  $\text{CH}_2\text{-CH}_2\text{-P}$ ); 4.51 (s, 2H, P-OH);

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ,  $\delta$ , ppm): 14.2 ( $\text{CH}_2\text{-CH}_3$ ); 21.9 ( $\text{CH}_2\text{-CH}_2\text{-P}$ ); 22.8 ( $\text{CH}_2\text{-CH}_3$ ); 24.0–29.6 ( $-\text{CH}_2-$ ); 30.4 ( $-\text{CH}_2\text{-P}$ ); 31.9 ( $\text{CH}_2\text{-CH}_2\text{-CH}_2\text{-P}$ );

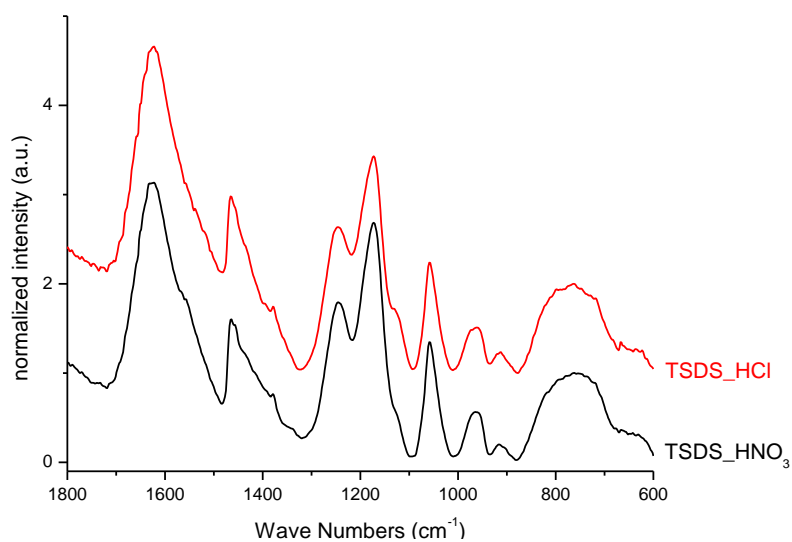
$^{31}\text{P}$  NMR ( $\text{CDCl}_3$ ,  $\delta$ , ppm): 38.0.

**Figure S1.** XRD of sol-gel synthesized titania nanoparticles.

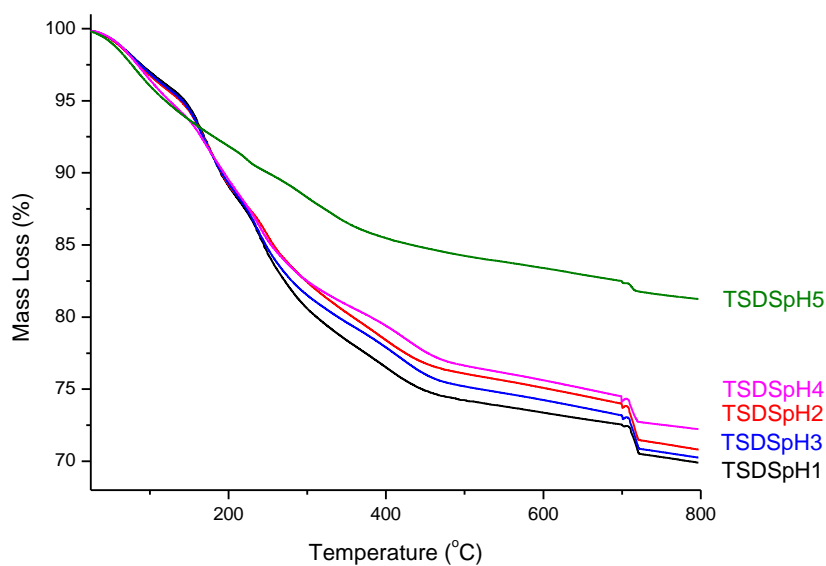


**Figure S2.** Dynamic light scattering (DLS) of titania nanoparticles.**Figure S3.** FT-IR of titania nanoparticles.**Figure S4.** FT-IR (3200–2800  $\text{cm}^{-1}$ ) of SDS@TiO<sub>2</sub> at pH 1, 2, 3, 4 and 5.

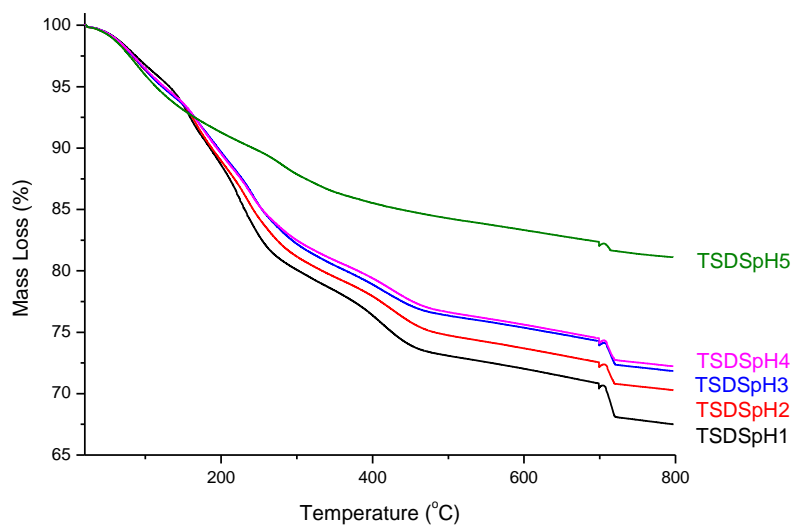
**Figure S5.** FT-IR (1800–600  $\text{cm}^{-1}$ ) of SDS@TiO<sub>2</sub> at pH 2, particles synthesized in HNO<sub>3</sub> or HCl respectively.

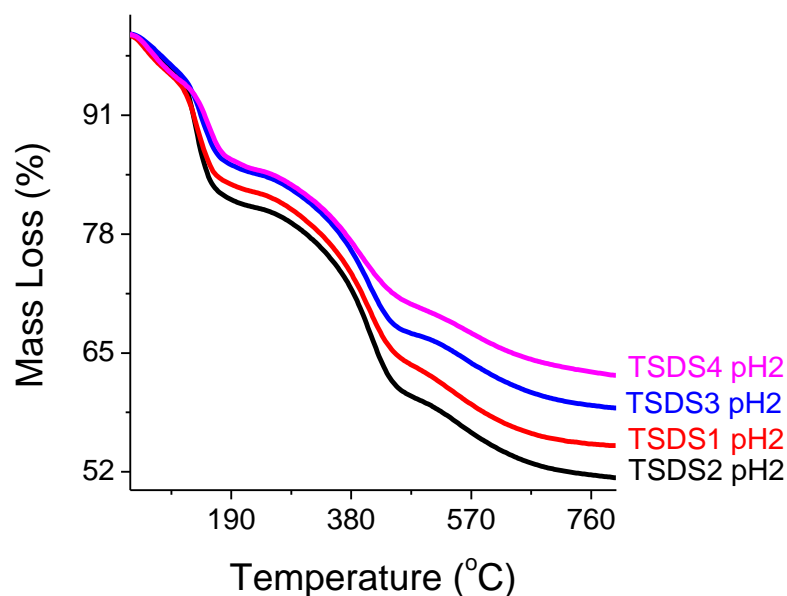


**Figure S6.** Thermograms of SDS@TiO<sub>2</sub> at pH 1, 2, 3, 4 and 5, particle synthesized in HNO<sub>3</sub>.



**Figure S7.** Thermograms of SDS@TiO<sub>2</sub> at pH 1, 2, 3, 4 and 5, particle synthesized in HCl.



**Figure S8.** Thermograms of titania SDS@TiO<sub>2</sub> at pH 2 with different concentrations of SDS.**Table S1.** Mass losses and surface coverage of SDS@TiO<sub>2</sub>, particles synthesized in HNO<sub>3</sub>.

| pH  | SDS Mass loss (%) | Surface coverage (Molecules/nm <sup>2</sup> ) |
|-----|-------------------|---|
| pH1 | 15.00             | 2.3   |
| pH2 | 14.45             | 2.3   |
| pH3 | 14.04             | 2.2   |
| pH4 | 13.80             | 2.2   |
| pH5 | 8.58              | 1.3   |

**Table S2.** Mass losses and surface coverage of SDS@TiO<sub>2</sub>, particles synthesized in HCl.

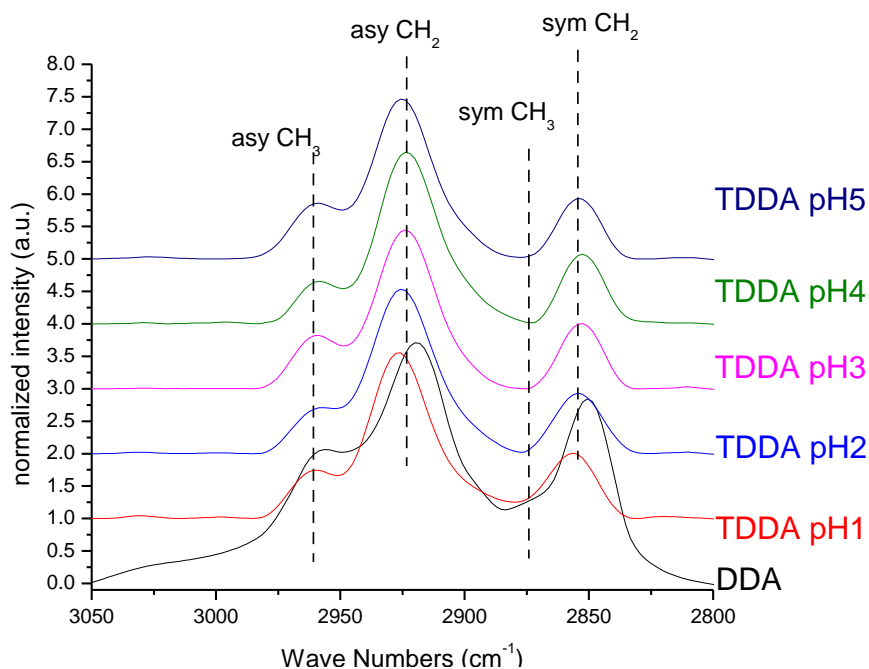
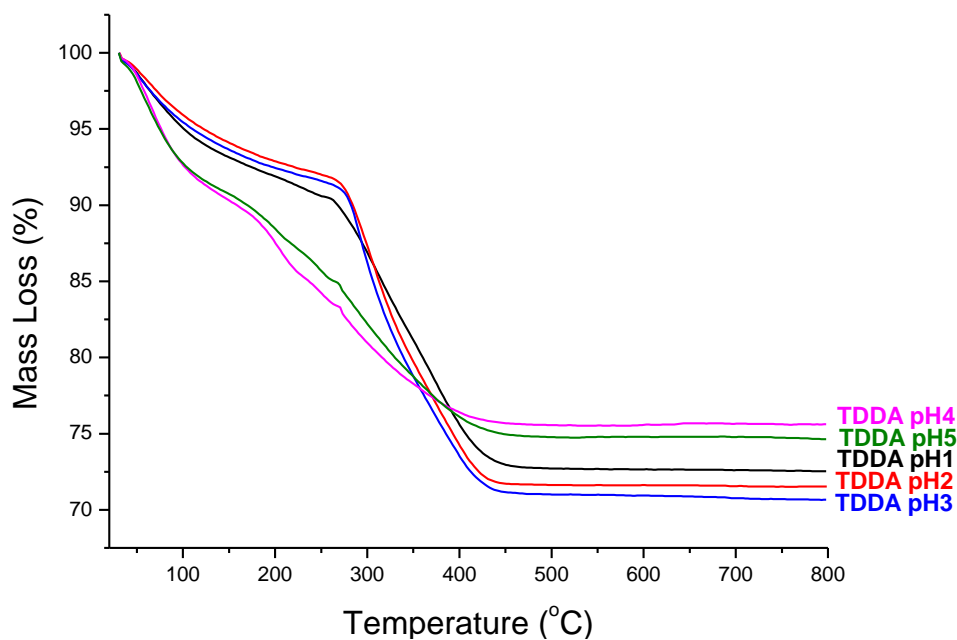
| pH  | SDS Mass loss (%) | Surface coverage (Molecules/nm <sup>2</sup> ) |
|-----|-------------------|---|
| pH1 | 15.95             | 2.5   |
| pH2 | 15.06             | 2.3   |
| pH3 | 14.15             | 2.2   |
| pH4 | 13.84             | 2.2   |
| pH5 | 8.60              | 1.3   |

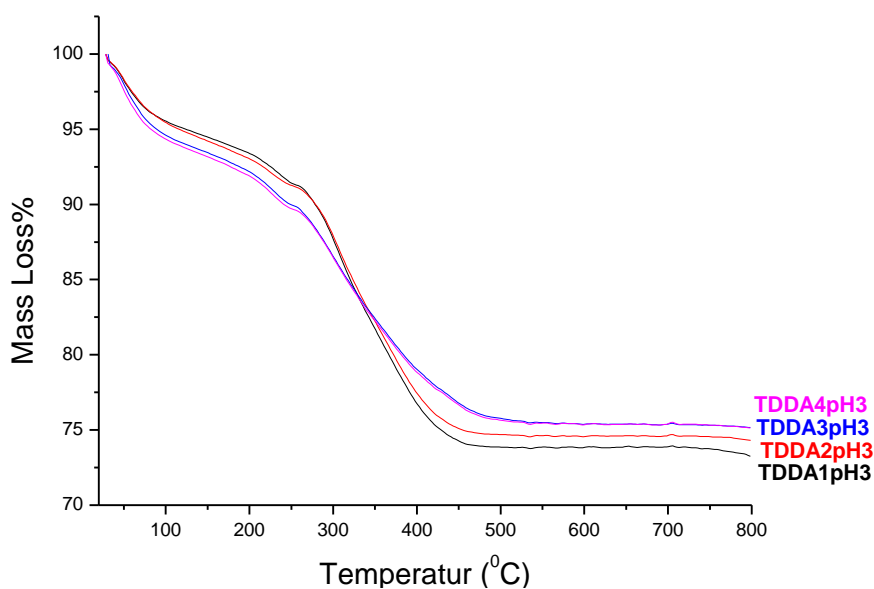
**Table S3.** Elemental Analyses of SDS@TiO<sub>2</sub> at pH 1, 2, 3, 4 and 5, particles synthesized in HNO<sub>3</sub>.

| No. | Sample ID                  | wt% C | wt% H | wt% N |
|-----|----------------------------|-------|-------|-------|
| 1   | SDS @ TiO <sub>2</sub> pH1 | 8.02  | 2.70  | 0.20  |
| 2   | SDS @ TiO <sub>2</sub> pH2 | 7.48  | 1.98  | 0.23  |
| 3   | SDS @ TiO <sub>2</sub> pH3 | 5.73  | 1.90  | 0.35  |
| 4   | SDS @ TiO <sub>2</sub> pH4 | 9.14  | 2.40  | 0.21  |
| 5   | SDS @ TiO <sub>2</sub> pH5 | 3.45  | 1.63  | 0     |

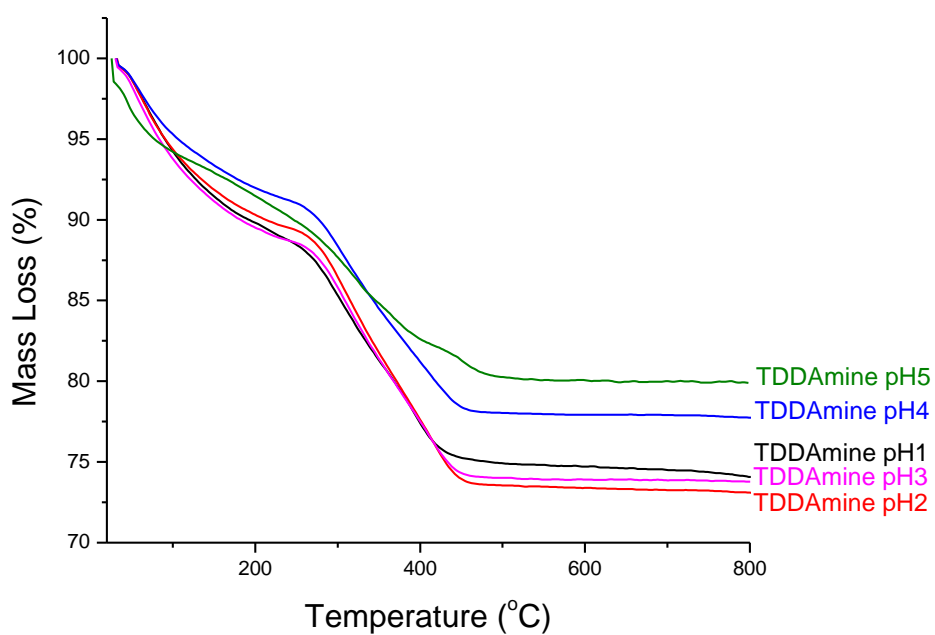
**Table S4.** Elemental Analyses of SDS@TiO<sub>2</sub> at pH 1, 2, 3, 4 and 5, particles synthesized in HCl.

| No. | Sample ID                  | wt% C | wt% H | wt% N |
|-----|----------------------------|-------|-------|-------|
| 1   | SDS @ TiO <sub>2</sub> pH1 | 11.27 | 2.70  | 0     |
| 2   | SDS @ TiO <sub>2</sub> pH2 | 9.52  | 2.47  | 0     |
| 3   | SDS @ TiO <sub>2</sub> pH3 | 8.98  | 2.43  | 0     |
| 4   | SDS @ TiO <sub>2</sub> pH4 | 8.98  | 2.41  | 0     |
| 5   | SDS @ TiO <sub>2</sub> pH5 | 2.92  | 1.71  | 0.12  |

**Figure S9.** FT-IR spectra (3050–2800 cm<sup>-1</sup>) of DDA@TiO<sub>2</sub> at pH 1, 2, 3, 4 and 5.**Figure S10.** TGA of DDA@TiO<sub>2</sub> at pH 1, 2, 3, 4 and 5.

**Figure S11.** TGA of DDA@TiO<sub>2</sub> at pH 3 with different concentrations of DDA.**Table S5.** Mass losses and surface coverage of DDA@TiO<sub>2</sub>.

| pH   | DDA Mass loss (%) | Surface coverage (Molecules/nm <sup>2</sup> ) |
|------|-------------------|---|
| pH 1 | 18.62             | 3.7   |
| pH 2 | 20.04             | 4.0   |
| pH 3 | 21.1              | 4.1   |
| pH 4 | 10.25             | 2.0   |
| pH 5 | 12.53             | 2.5   |

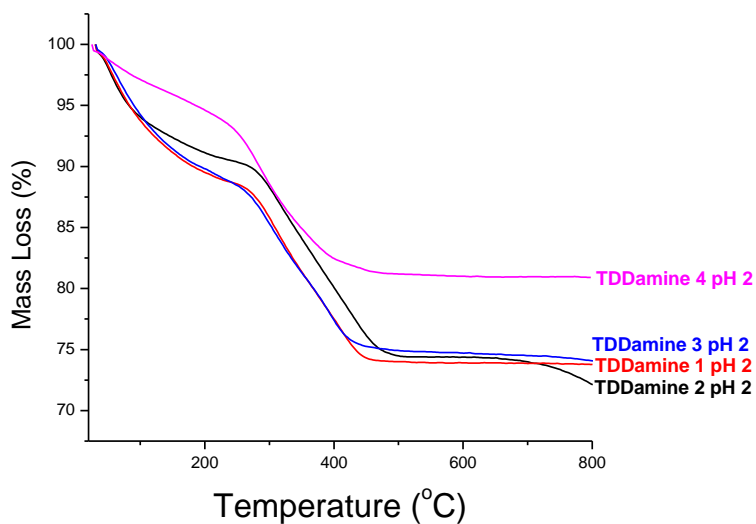
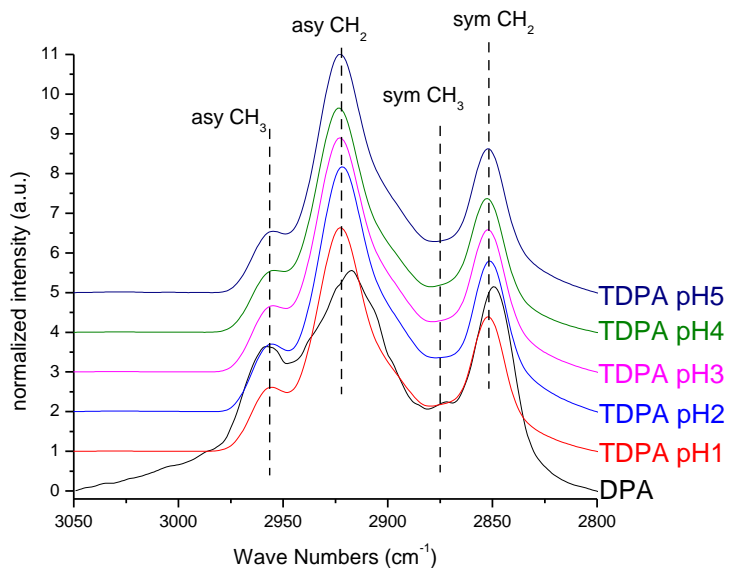
**Figure S12.** TGA of DDAmine@TiO<sub>2</sub> at pH 1, 2, 3, 4 and 5.

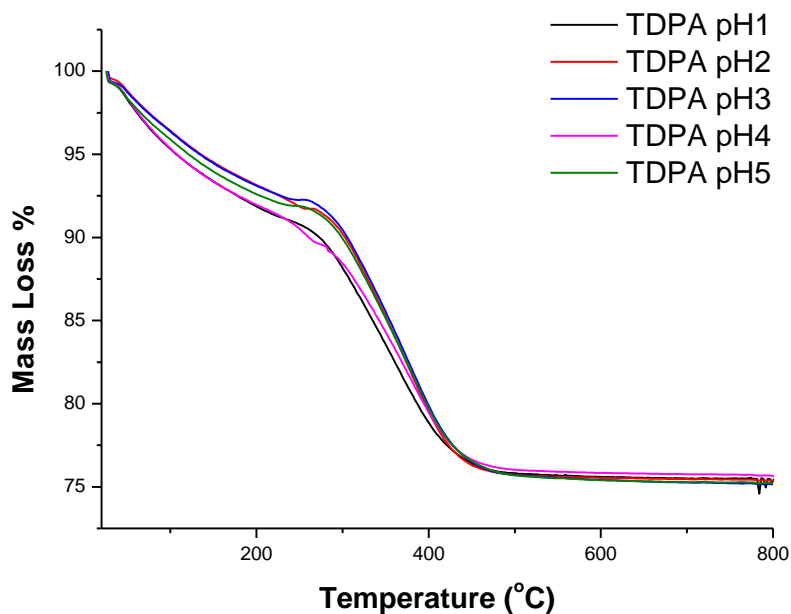
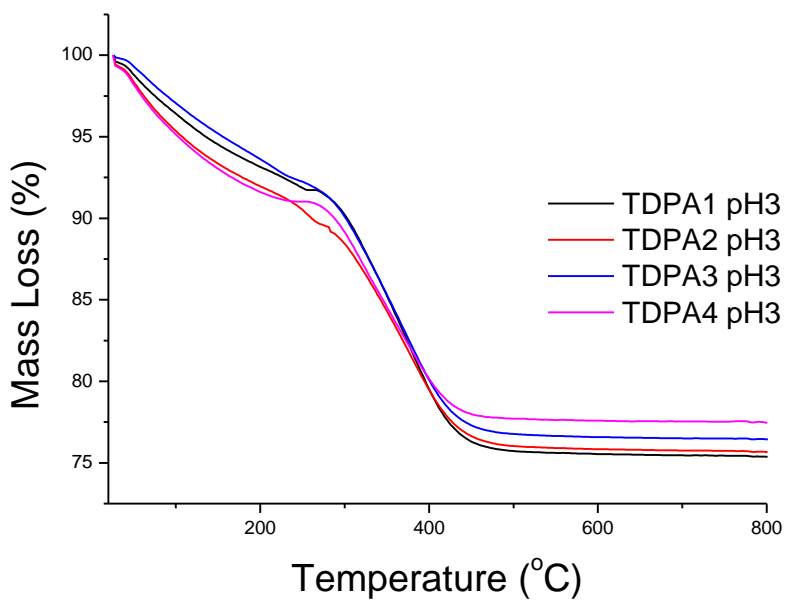
**Table S6.** Elemental analysis of DDAmine@TiO<sub>2</sub> at pH 1, 2, 3, 4 and 5.

| Sample       | wt% C | wt% H | wt% N |
|--------------|-------|-------|-------|
| TDDAmine pH1 | 11.10 | 2.50  | 0.95  |
| TDDAmine pH2 | 12.13 | 2.91  | 1.18  |
| TDDAmine pH3 | 11.52 | 2.32  | 0.89  |
| TDDAmine pH4 | 10.6  | 2.40  | 1.09  |
| TDDAmine pH5 | 7.33  | 1.81  | 0.81  |

**Table S7.** Mass losses and surface coverage of DDAmine@TiO<sub>2</sub>.

| pH   | DDAmine Mass loss (%) | Surface coverage (Molecules/nm <sup>2</sup> ) |
|------|-----------------------|---|
| pH 1 | 14.54                 | 3.3   |
| pH 2 | 16.37                 | 3.7   |
| pH 3 | 15.2                  | 3.4   |
| pH 4 | 13.57                 | 3.1   |
| pH 5 | 10.13                 | 2.3   |

**Figure S13.** TGA of DDAmine@TiO<sub>2</sub> at pH 2 with different concentrations of DDAmine.**Figure S14.** FT-IR spectra of DPA@TiO<sub>2</sub> at pH 1, 2, 3, 4 and 5.

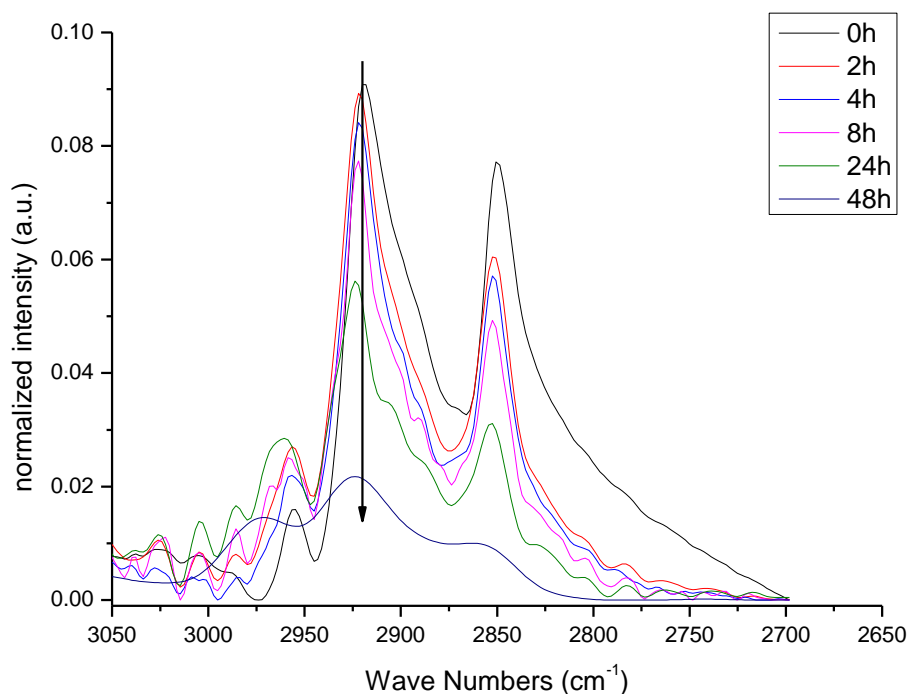
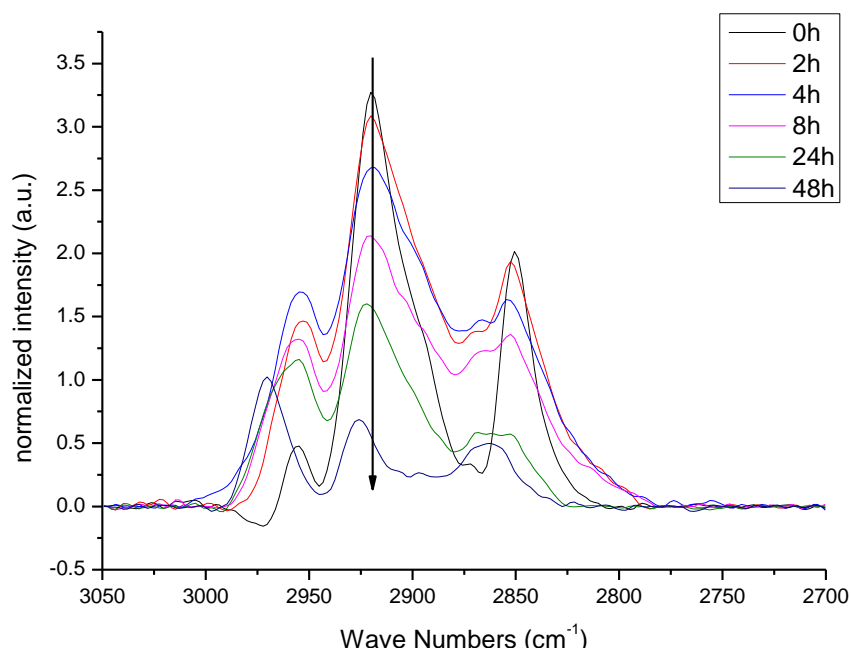
**Figure S15.** TGA of DPA@TiO<sub>2</sub> at pH1 to pH5.**Figure S16.** Thermograms of DPA@TiO<sub>2</sub> with different concentrations of DPA at pH3.**Table S6.** Elemental analyses of DPA@TiO<sub>2</sub> at pH = 1 to pH = 5.

| Sample    | wt% C | wt% H | wt% P |
|-----------|-------|-------|-------|
| TDPA pH 1 | 9.28  | 1.72  | 0.849 |
| TDPA pH 2 | 11.13 | 2.85  | 1.03  |
| TDPA pH 3 | 11.58 | 2.91  | 1.18  |
| TDPA pH 4 | 9.59  | 2.32  | 1.08  |
| TDPA pH 5 | 8.33  | 2.01  | 0.90  |

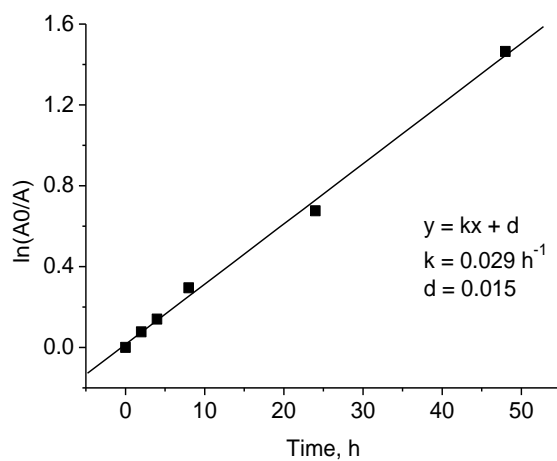


**Table S7.** Mass loss and surface coverage of DPA@TiO<sub>2</sub>.

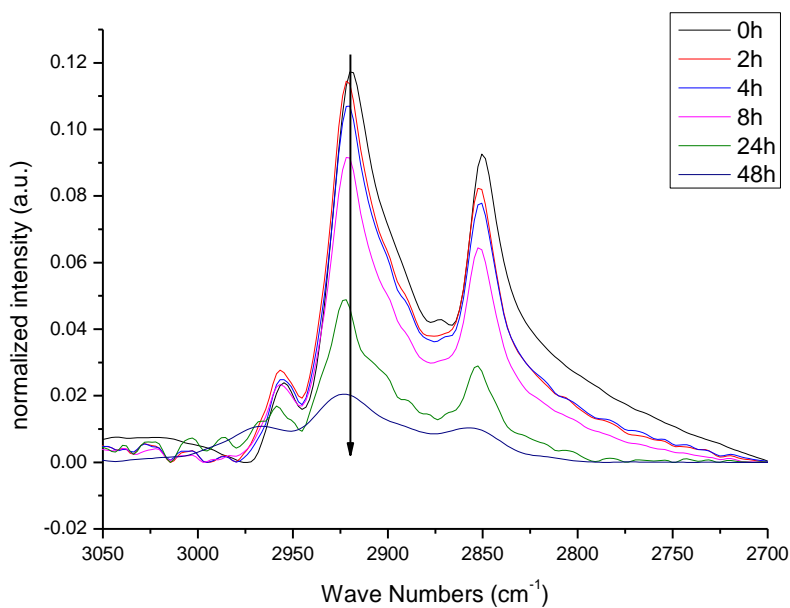
| pH   | DPA Mass loss (%) | Surface coverage (Molecules/nm <sup>2</sup> ) |
|------|-------------------|---|
| pH 1 | 15.5              | 3.8   |
| pH 2 | 16.2              | 4.0   |
| pH 3 | 16.7              | 4.1   |
| pH 4 | 15.3              | 3.7   |
| pH 5 | 14.7              | 3.6   |

**Figure S17.** FT-IR spectra (KBr: 2 mg sample, 150 mg KBr) of SDS@TiO<sub>2</sub> after different times of illumination, particles synthesized in HNO<sub>3</sub>.**Figure S18.** FT-IR spectra (KBr: 2 mg sample, 150 mg KBr) of SDS@TiO<sub>2</sub> after different times of illumination, particles synthesized in HCl.

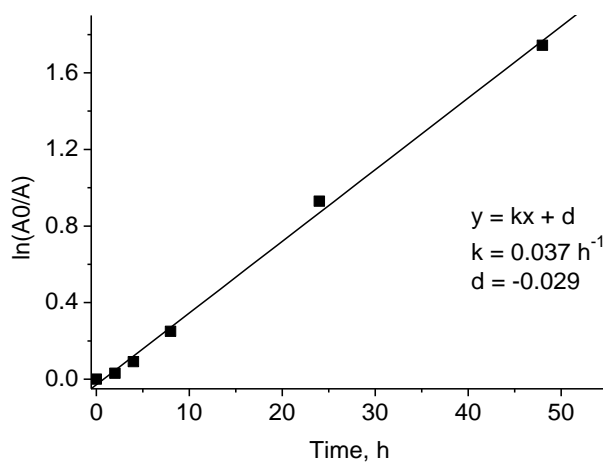
**Figure S19.** Kinetic plot for determining the first-order reaction rate constant  $k$  of SDS@TiO<sub>2</sub>.



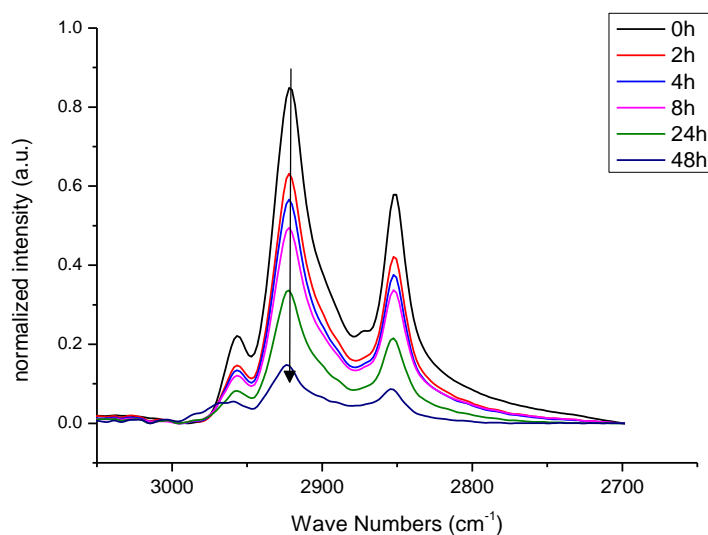
**Figure S20.** FT-IR spectra (KBr: 2 mg sample, 150 mg KBr) of DDA@TiO<sub>2</sub> after different times of illumination.



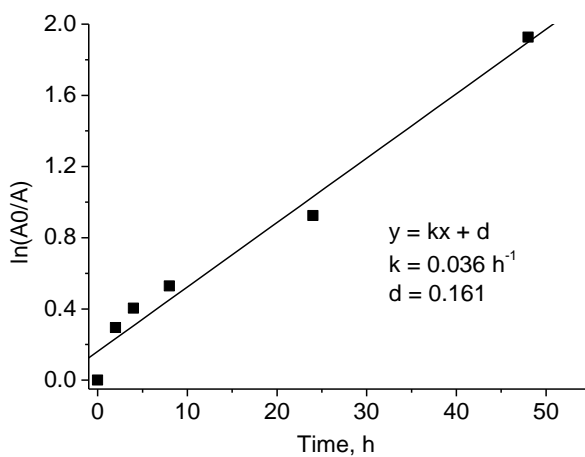
**Figure S21.** Kinetic plot for determining the first-order reaction rate constant  $k$  of DDA@TiO<sub>2</sub>.



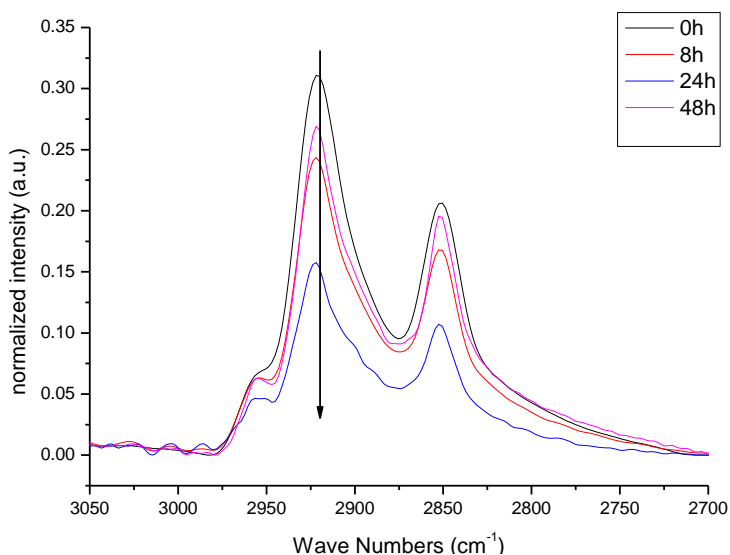
**Figure S22.** FT-IR spectra (KBr: 2 mg sample, 150 mg KBr) of DDAmine@TiO<sub>2</sub> after different times of illumination.



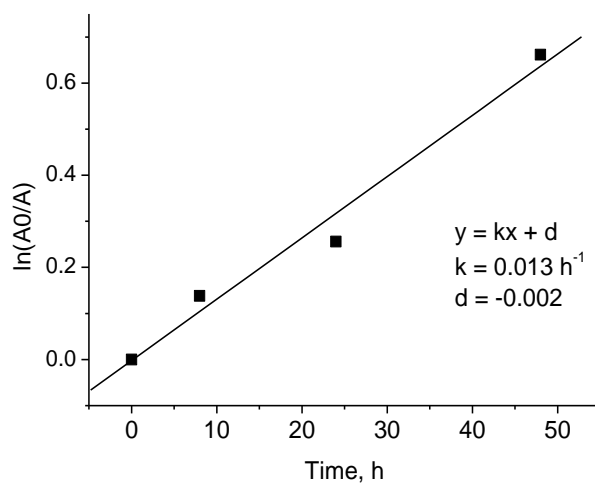
**Figure S23.** Kinetic plot for determining the first-order reaction rate constant  $k$  of DDAmine@TiO<sub>2</sub>.



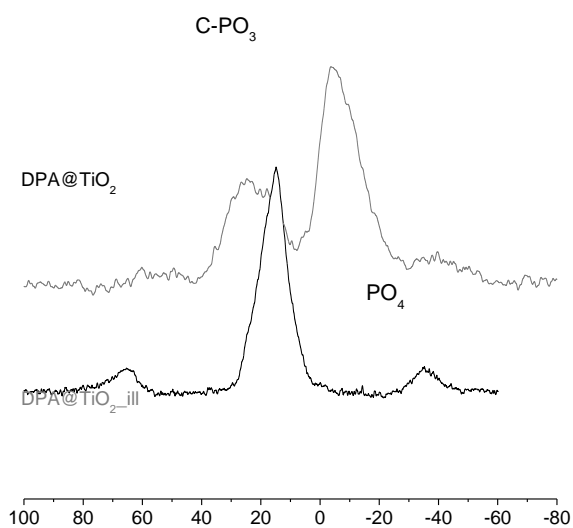
**Figure S24.** FT-IR spectra (KBr: 2 mg sample, 150 mg KBr) of DPA@TiO<sub>2</sub> after different times of illumination.



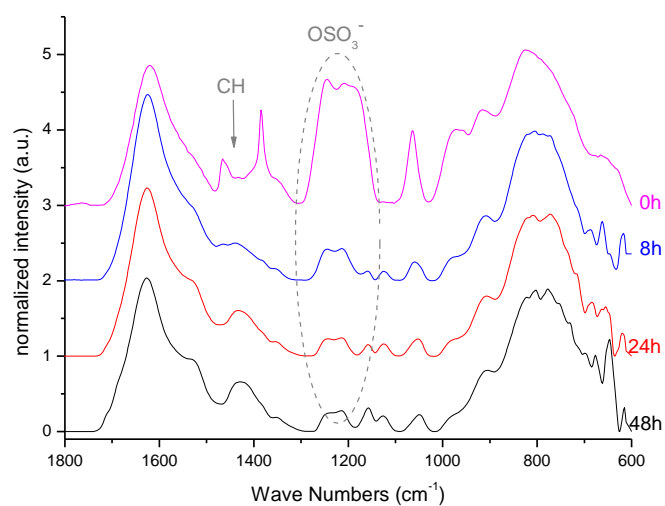
**Figure S25.** Kinetic plot for determining the first-order reaction rate constant  $k$  of DPA@TiO<sub>2</sub>.



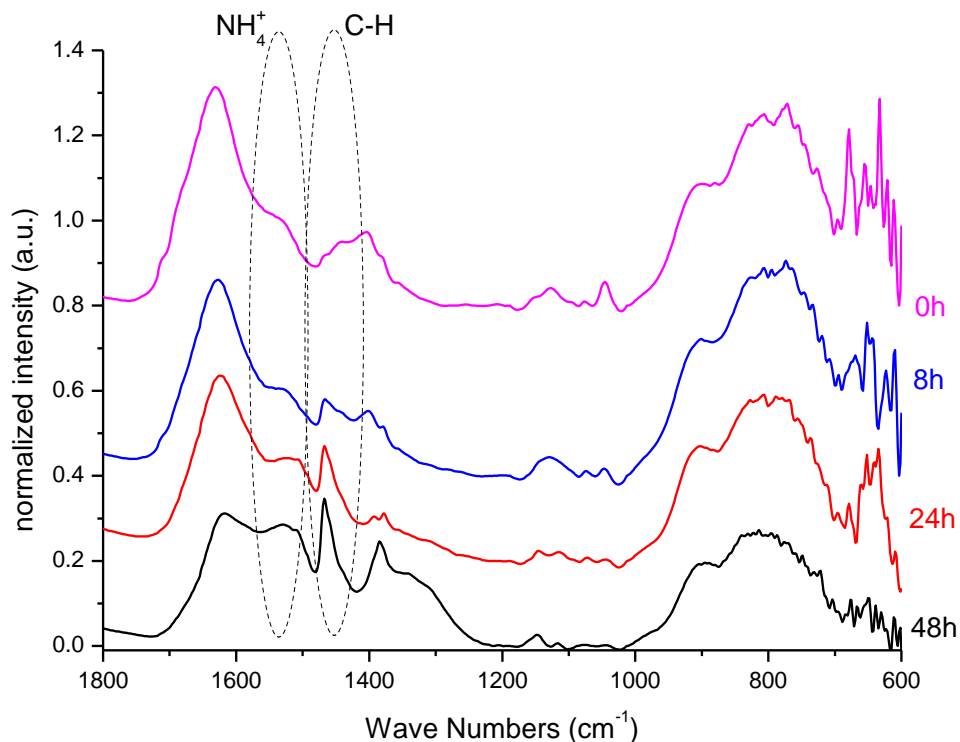
**Figure S26.** <sup>31</sup>P MAS NMR spectra of DPA@TiO<sub>2</sub> without illumination and after 16 days of illumination.



**Figure S27.** FT-IR spectra (KBr: 2 mg sample, 150 mg KBr) of SDS@TiO<sub>2</sub> after different times of illumination.



**Figure S28.** FT-IR spectra (KBr: 2 mg sample, 150 mg KBr) of DDAmine@TiO<sub>2</sub> after different times of illumination.



**Figure S29.** FT-IR spectra (1600–700 cm<sup>-1</sup>) of SDS@TiO<sub>2</sub> functionalized at pH 1, 2, 3, 4 and 5 in HCl.

