Facet-Dependent Interfacial Charge Transfer in TiO_2/Nitrogen-Doped Graphene Quantum Dots Heterojunctions for Visible Light Driven Photocatalysis

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Figures

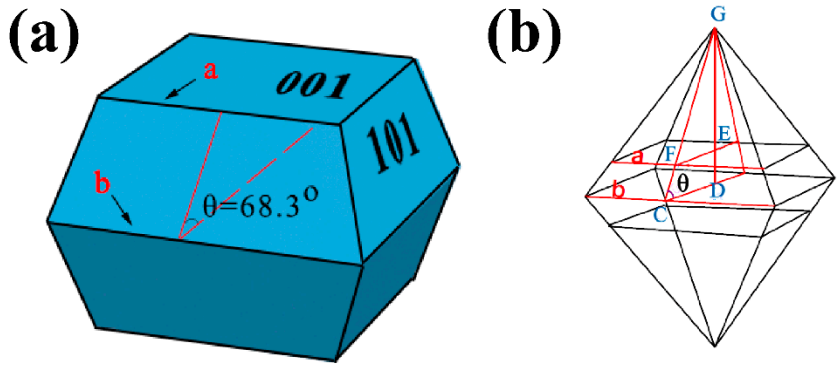

Figure S1. (**a**) Slab model of anatase TiO_2 single crystal, and (**b**) equilibrium model of anatase TiO_2 single crystal.

Calculation method of the percentage of {001} facets, based on previously reported literature [2-5]:

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

$$S_{101} = 8\left(\frac{1}{2}CG * b - \frac{1}{2}GF * a\right)$$

$$S_{001}\% = \frac{S_{001}}{S_{001} + S_{101}}$$

$$= \frac{2a^2}{2a^2 + 8\left(\frac{1}{2}CG * b - \frac{1}{2}GF * a\right)}$$

$$= \frac{a^2}{a^2 + 4\left(\frac{1}{2} * \frac{\frac{1}{2}b}{cos\theta} * b - \frac{1}{2}\frac{\frac{1}{2}a}{cos\theta} * a\right)}$$

$$= \frac{a^2}{a^2 + \frac{b^2 - a^2}{cos\theta}} = \frac{1}{1 + \frac{\frac{b^2}{a^2} - 1}{cos\theta}}$$

$$= \frac{cos\theta}{cos\theta + \frac{b^2}{a^2} - 1} \quad (1)$$

Herein, two independent parameters b and a denote the lengths of the side of the bipyramid and the side of the square {001} 'truncation' facets, respectively. θ is the theoretical value (68.3°) for the angle between the {001} and {101} facets of anatase.

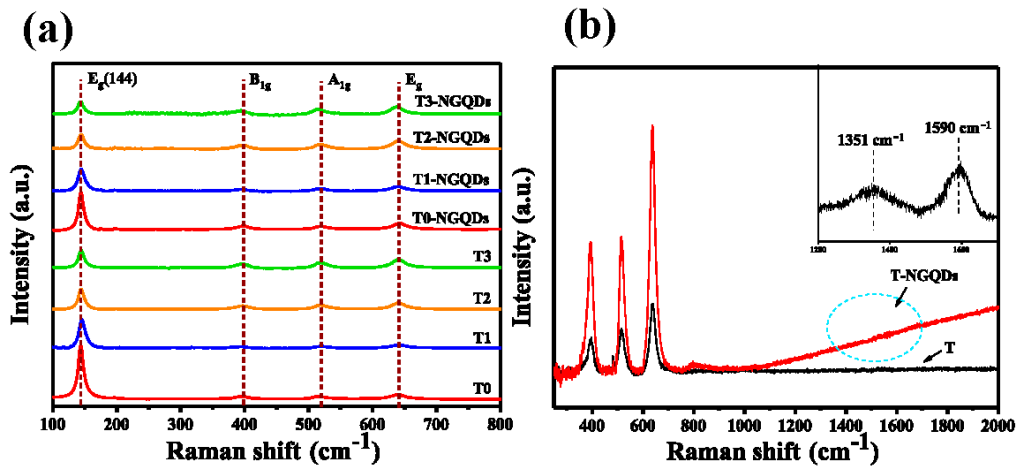

Figure S2. (**a**) Raman spectra of different TiO_2 samples without and with NGQDs decoration. (**b**) Raman spectra of T1 before and after decoration of NGQDs. The inset in Figure S2b is the enlargement of 1200–1700 cm^{-1} of T1-NGQDs.

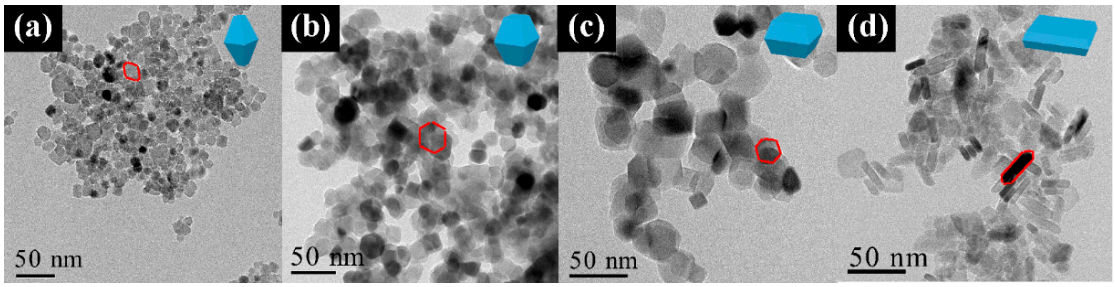

Figure S3. TEM images of (**a**) T0, (**b**) T1, (**c**) T2, and (**d**) T3.

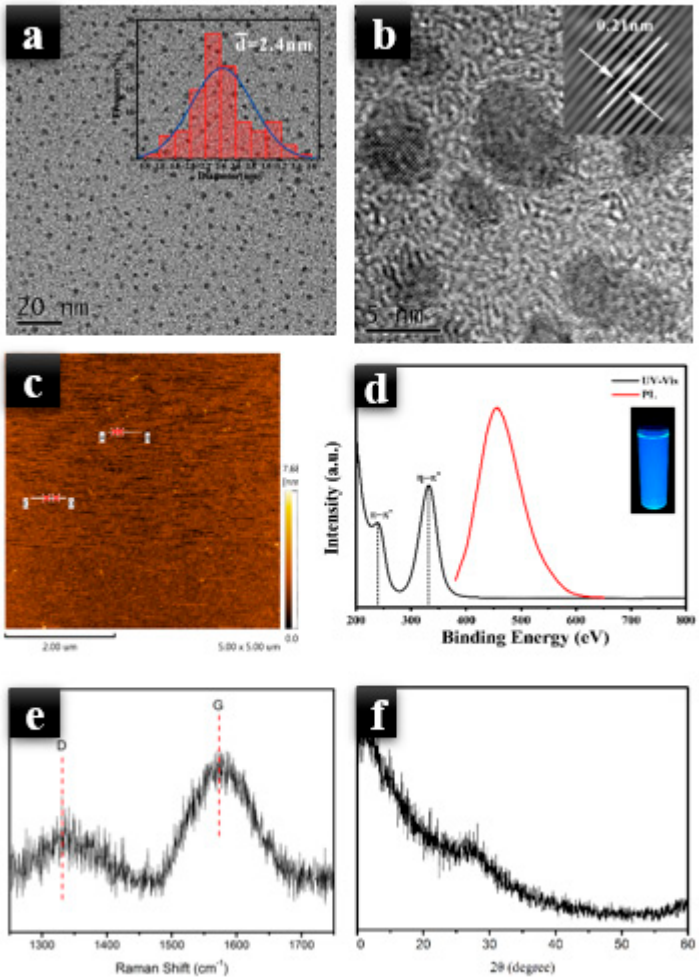

Figure S4. (**a**) TEM image, (**b**) HRTEM image, (**c**) AFM image, (**d**) UV-vis spectra and PL spectra of the GQDs (the excitation wavelength is 365 nm), (**e**) Raman spectra and (**f**) XRD pattern of NGQDs. The inset in (**a**) is the size distribution of NGQDs. The inset in (**b**) is the autocorrelated HRTEM lattice images.

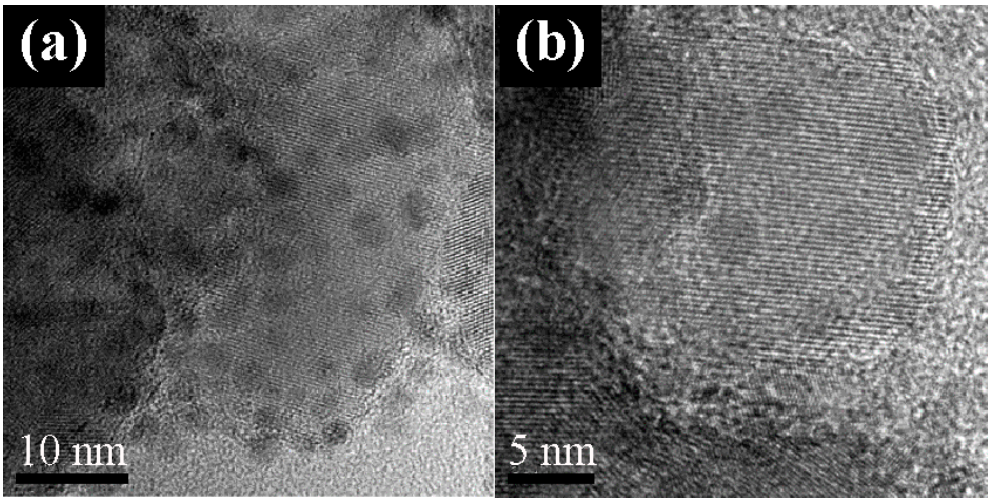

Figure S5. HRTEM images of the anatase TiO_2 decorate with NGQDs.

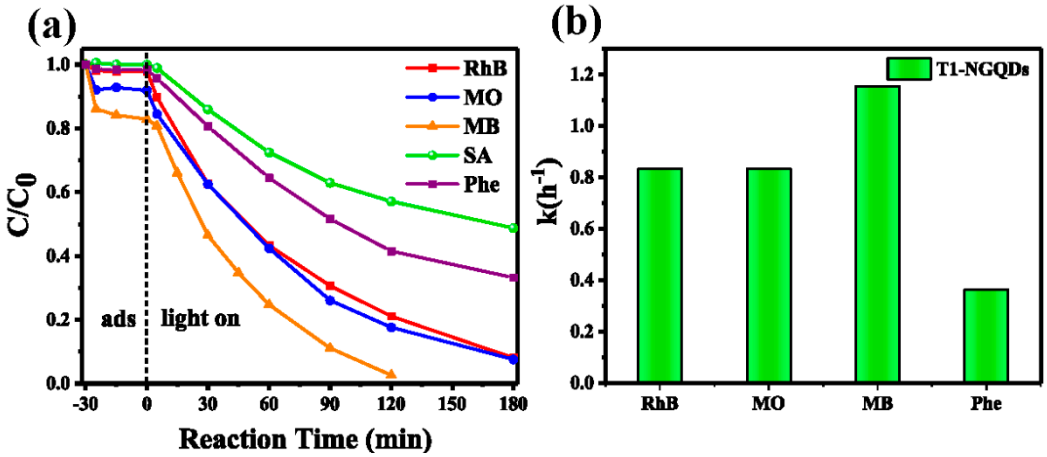

Figure S6. (**a**) The photocatalytic degradation of different pollutants for T1-NGQDs, and (**b**) plot of k values for different pollutants degradation in T1-NGQDs.

References

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