Electronic Supplementary Information

Supporting Information

Enhanced UV-Visible Lights Photodetectors with TiO_2/Si Heterojunction through Band Engineering

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Part I: Calculations

1. Depletion layer width and capacitance calculation of double Schottky structure

In the heterojunction structure of the undoped TiO_2/Si and In-doped TiO_2/Si, the depletion layer widths have two major regions, i.e., W_{Si} in Si and W_{TO} in TiO_2, as shown in **Figure S1**. According to the unilateral mutation junction model, their thicknesses can be obtained using the Poisson equation as follows:

$$W_{Si} = \sqrt{\frac{2\varepsilon_{Si}}{qN_{D1}}(\varphi_{bi1} - V_1 - \frac{kT}{q})} \quad \text{(S1)}$$

$$W_{TO} = \sqrt{\frac{2\varepsilon_{TO}}{qN_{D2}}(\varphi_{bi2} - V_2 - \frac{kT}{q})} \quad \text{(S2)}$$

Where *k, T* are the Boltzmann constant and temperature, ε_{Si} and ε_{TO} are the static dielectric values of Si and TiO_2, N_{D1} and N_{D2} represent the impurity concentrations in Si and TiO_2, φ_{bi1} and φ_{bi2} represent the built-in potential of two semiconductors, respectively. The applied bias is V (equal to $V_1 + V_2$). The depletion layer capacitance C_{D1} and C_{D2} are shown as follows:

$$C_{D1} = \frac{\varepsilon_{Si}}{W_{Si}} = \sqrt{\frac{q\varepsilon_{Si}N_{D1}}{2(\varphi_{bi1} - V_1 - \frac{kT}{q})}} \quad \text{(S3)}$$

$$C_{D2} = \frac{\varepsilon_{TO}}{W_{TO}} = \sqrt{\frac{q\varepsilon_{TO}N_{D2}}{2(\varphi_{bi2} - V_2 - \frac{kT}{q})}} \quad \text{(S4)}$$

The total capacitance for the heterojunction is the series of two capacitors, as suggested by this equation:

$$\frac{1}{C} = \frac{1}{C_{D1}} + \frac{1}{C_{D2}} = \sqrt{\frac{2(\varphi_{bi1} - V_1 - \frac{kT}{q})}{q\varepsilon_{Si}N_{D1}}} + \sqrt{\frac{2(\varphi_{bi2} - V_2 - \frac{kT}{q})}{q\varepsilon_{TO}N_{D2}}} \quad \text{(S5)}$$

The capacitance of a unilateral linearly graded junction [10] (C_{D3}) is given as follows:

$$C_{D3} = \frac{\varepsilon_{TO} S}{W_{TO}} = \left[\frac{q a \varepsilon_{TO}{}^{2}}{12(\varphi_{bi} - V)} \right]^{1/3} S \qquad \text{(S6)}$$

Where a is the constant of N doping concentration gradient and φ_{bi} is the built-in potential (very small).

The function logarithmic form is given as follows:

$$\log(C) \approx -\frac{1}{3}\log(-V) + \mathrm{C} \qquad \text{(S7)}$$

2. The responsivity (R) and quantum efficiency (η) of n-Si/TiO_2 heterojunction are calculated by the following two equations:

$$R = \frac{I_{photo}}{PA} \qquad \text{(S8)}$$

$$G\eta = \frac{I_{photo}/q}{PA/h\nu} \qquad \text{(S9)}$$

where *I, P,G, A, h* and ν are the photocurrent density, light energy density, internal gain, area of the device, Planck's constant and photon frequency, respectively.

The photocurrent I_{photo} could be calculated by this equation:

$$I_{photo} = I - I_{dark} \qquad \text{(S10)}$$

The ratio of the photocurrent/dark current could be calculated by the following equation:

$$Ratio = \frac{I - I_{dark}}{I_{dark}} \qquad \text{(S11)}$$

where I and I_{dark} are the electric currents measured from the device under the illumination and dark, respectively.

3. The multiplication factor (M_{ph}) was calculated by the following equation:

$$M_{ph} = \sqrt{\frac{V_B}{nI_{ph}R_s}} \quad \text{(S12)},$$

where V_B is the applied bias, I_{ph} is the current of transited photo-generated carriers without multiplying, R_s is the equivalent series resistance of device, n is constant depended on the semiconductor and the doping profile and the wavelength of the incident light, respectively.

References

[1] S. M. Sze, *Physics of Semiconductor Devices*, 2nd ed (Wiley, New York, **1981**).

[2] E. A. Kraut, R. W. Grant, J. R. Waldrop, S. P. Eowalczyk, *Phys. Rev. Lett.* **1980**, 44, 1620.

[3] H.Melchior, W.T. Lynch,*IEEE Trans. on Electron Dev.* **1966**, ED-13, 829.

Part II: Supplementary Figures

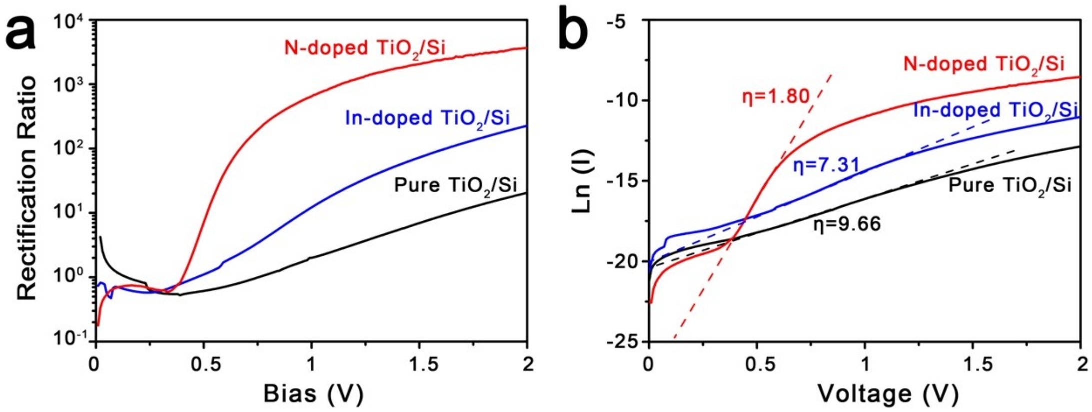

Figure S1. (a) The rectification ratios of the undoped TiO_2/Si, In-doped TiO_2/Si and N-doped TiO_2/Si heterojunctions with the bias of 0 V to 2 V. (b) In(*I*)-*V* characteristics of those heterojunctions with forward voltage from 0 V to 2 V.

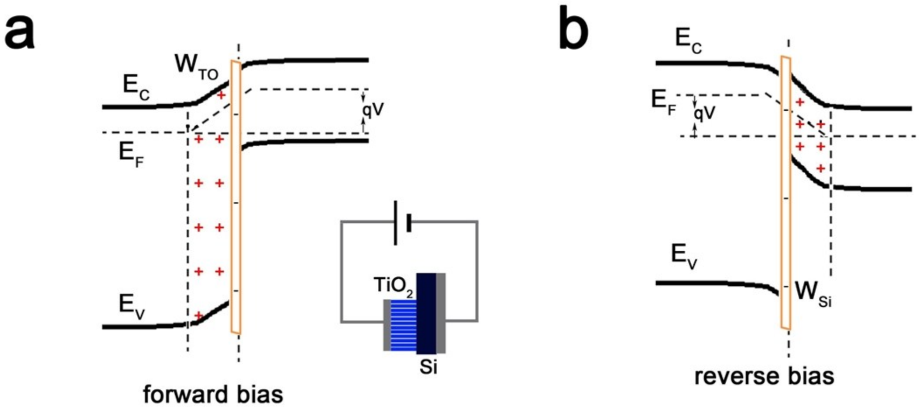

Figure S2. Schematic representation of the band energies and internal electrical field of the TiO_2/Si heterojunctions with forward bias (a) and reverse bias (b), respectively.

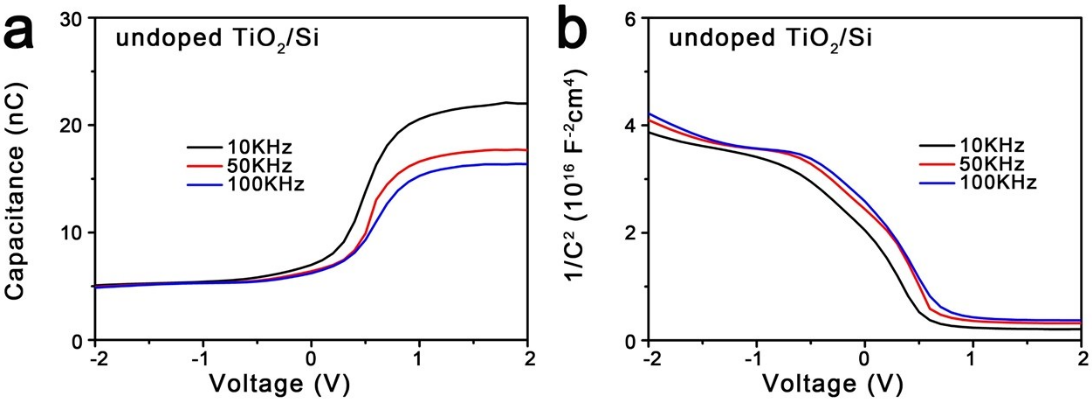

Figure S3. The capacitance-voltage characteristic (a) and $1/C^2$ versus V plots (b) of the undoped TiO_2/Si heterojunctions, measured in the dark at the frequencies of 10 kHz, 50 kHz and 100 kHz at room temperature.

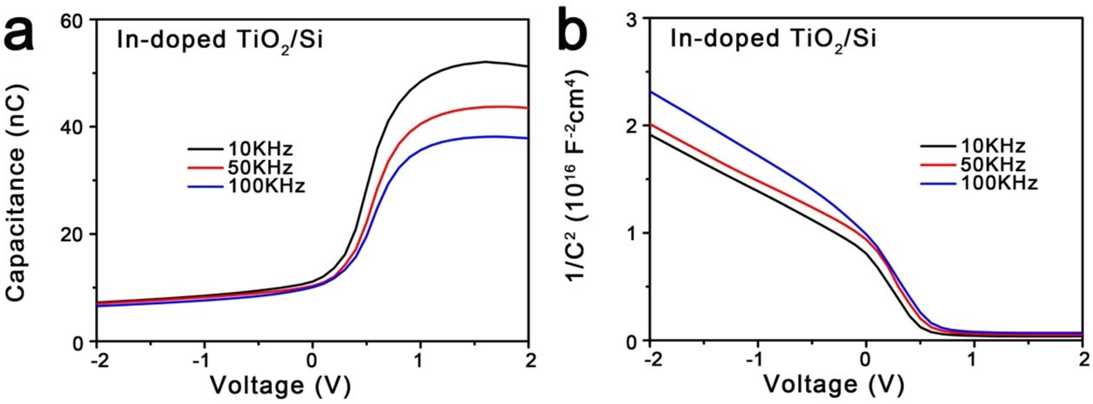

Figure S4. The capacitance-voltage characteristic (a) and $1/C^2$ versus V plots (b) of the In-doped TiO_2/Si heterojunctions, measured in the dark at the frequencies of 10 kHz, 50 kHz and 100 kHz at room temperature.

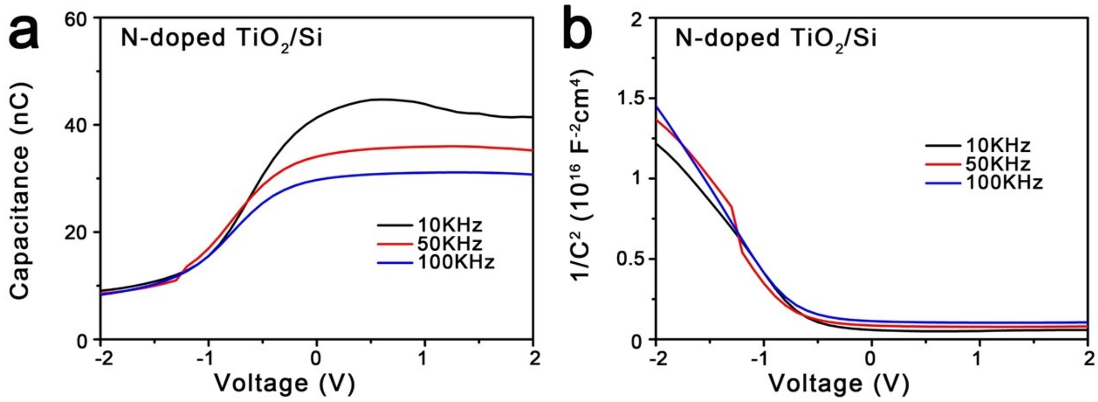

Figure S5. The capacitance-voltage characteristic (a) and $1/C^2$ versus V plots (b) of the N-doped TiO_2/Si heterojunctions, measured in the dark at the frequencies of 10 kHz, 50 kHz and 100 kHz at room temperature.

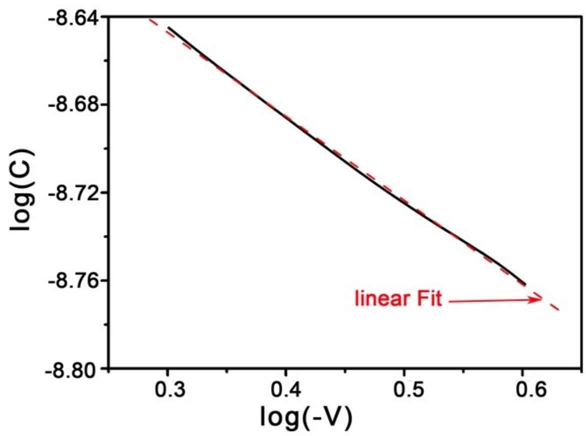

Figure S6. The log (C) versus log (-V) plots and linearly fitted at 10 kHz at room temperature.

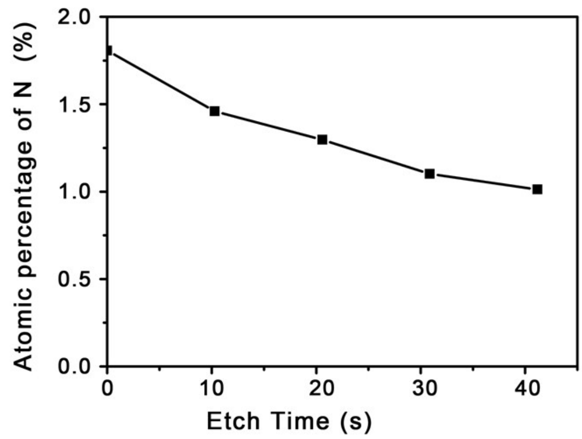

Figure S7. The relationship between the percentage of N atoms and the etching time.

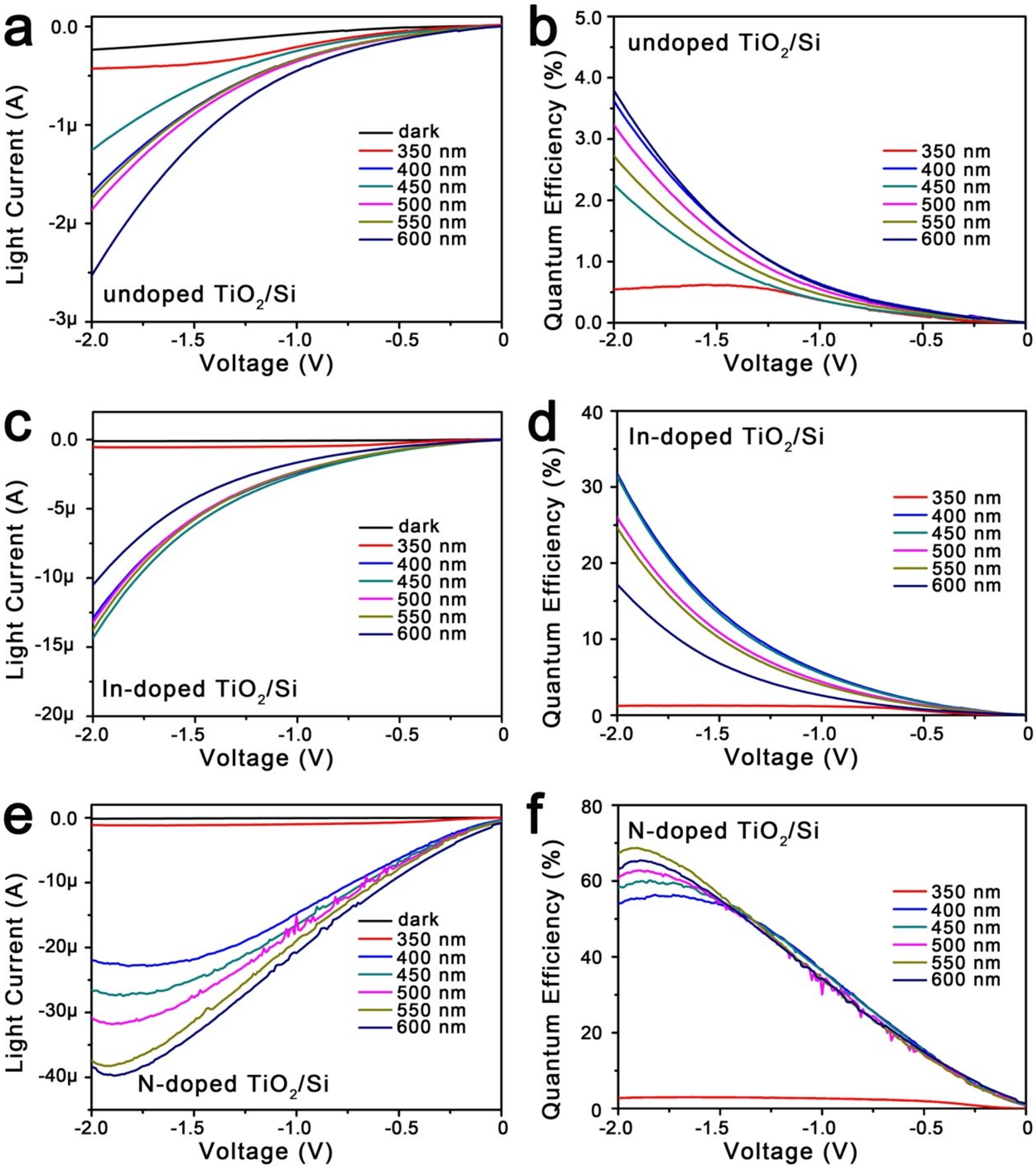

Figure S8. The light I-V curves (a, c and e) and the converted quantum efficiency (b, d and f) of the undoped TiO_2/Si, In-doped TiO_2/Si and N-doped TiO_2/Si heterojunctions at a reverse bias under dark, 350 nm, 400 nm, 450 nm, 500 nm, 550 nm and 600 nm, respectively. Here, the light intensity is 0.5 mW/cm^2.

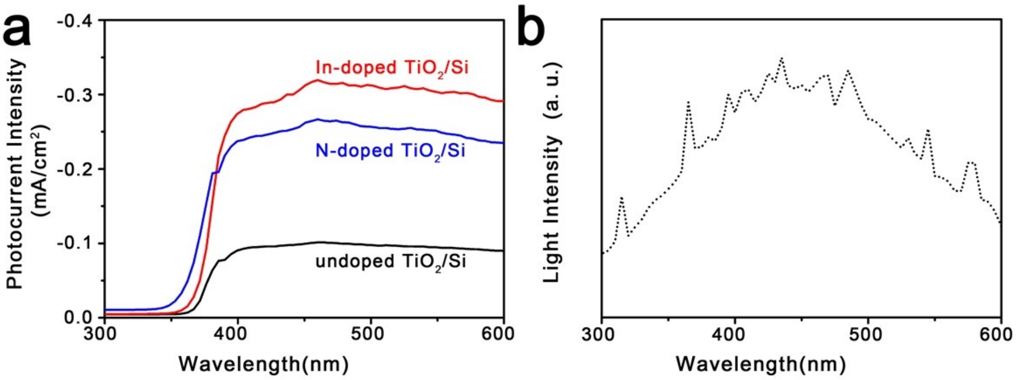

Figure S9. (a) The photocurrent spectra of the undoped TiO_2/Si, In-doped TiO_2/Si and N-doped TiO_2/Si heterjunctions with an applied reverse bias of -2 V. (b) Light intensity distribution along the wavelength of Xenon lamp.

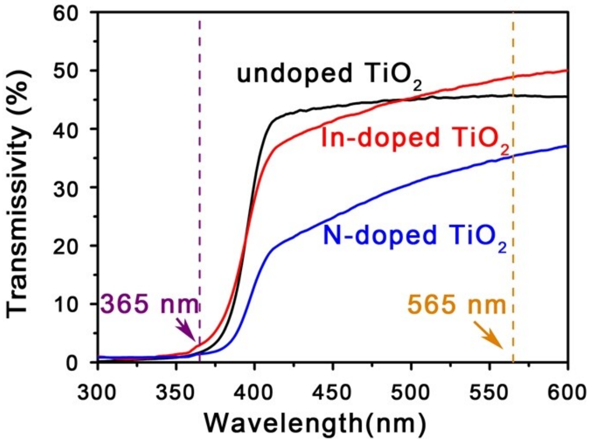

Figure S10. The transmittance of the undoped TiO_2, In-doped TiO_2 and N-doped TiO_2 from 300 nm to 600 nm.

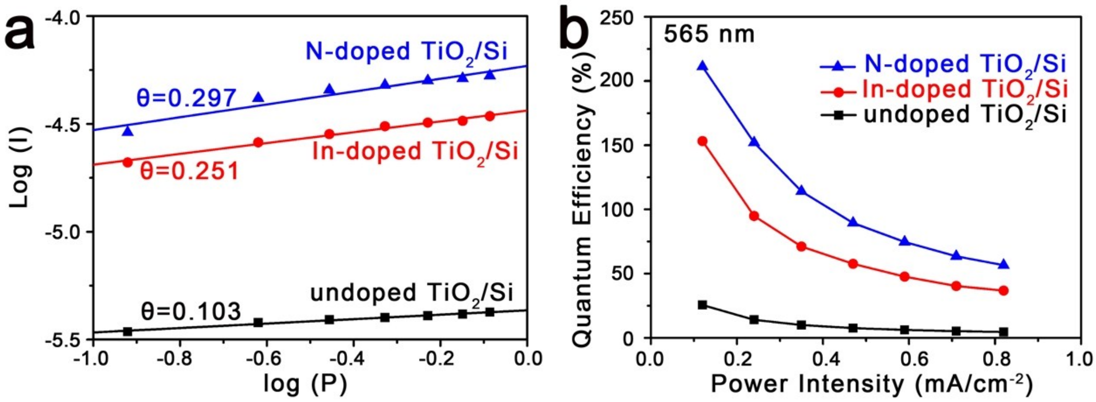

Figure S11. The logarithmic form of the photocurrent vs light power intensity (a) and the quantum efficiency (b) at -2 V for the undoped TiO_2/Si, In-doped TiO_2/Si and N-doped TiO_2/Si heterojunctions under 565 nm light illumination, respectively.