Supplementary Information

Unveiling the enhanced photoelectrochemical and photocatalytic properties of reduced graphene oxide for photodegradation of methylene blue dye

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Description of Supplementary Information

**Fig. S1.** Light spectrum of UV-C light source for photodegradation experiment.

**Fig. S2.** Tauc plot for indirect band gap of G-0 to G-8.

**Fig. S3.** 50 ppm MB for photolysis, and dark adsorption by G-0 to G-8.

**Fig. S4.** Time-dependent UV-Vis absorption spectra for photodegradation of 50 ppm MB from time 0 to 6 h by (a) G-0, (b) G-1, (c) G-2, (d) G-4, and (e) G-8.

**Eqn (S1).** Conversion of vs. Ag/AgCl pH 6.5 to vs. NHE pH 7.0.

**Eqn (S2).** Calculation of acceptor charge density of p-type semiconductor.

**Eqn (S3).** Calculation of conduction band potential.
**Fig. S1.** Light spectrum of UV-C light source for photodegradation experiment.
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Fig. S3. 50 ppm MB for photolysis, and dark adsorption by G-0 to G-8.
Fig. S4. Time-dependent UV-Vis absorption spectra for photodegradation of 50 ppm MB from time 0 to 6 h by (a) G-0, (b) G-1, (c) G-2, (d) G-4, and (e) G-8.
Eqn (S1). Conversion of vs. Ag/AgCl pH 6.5 to vs. NHE pH 7.0.

Conversion of potential, $E$ from versus Ag/AgCl (pH 6.5) to versus normal hydrogen electrode (NHE, pH 7) [1].

$$E_{\text{NHE, pH 7}} = E_{(\text{Ag/AgCl pH 6.5})} + 0.21 - 0.059 \times (7.0 - 6.5)$$  \hspace{1cm} (S1)
Eqn (S2). Calculation of acceptor charge density of p-type semiconductor.

\[
\frac{1}{C^2} = \frac{2}{\varepsilon \varepsilon_0 N_A} \left[ (-V + E_{FB}) - \frac{kT}{e} \right]
\]

\[
\frac{1}{C^2} = \frac{2}{\varepsilon \varepsilon_0 N_A} [-V + E_{FB}]
\]

\[
\frac{1}{C^2} \frac{dV}{dV} = \frac{2}{\varepsilon \varepsilon_0 N_A}
\]

\[
-\text{gradient} = \frac{2}{\varepsilon \varepsilon_0 N_A}
\]

\[
N_A = -\frac{2}{\varepsilon \varepsilon_0 (\text{gradient})} \frac{kT}{e}
\]

The value of \( \frac{kT}{e} \) is negligibly small at room temperature [2]. The M-S plot is \( 1/C^2 \) (y-axis) versus V (x-axis), hence \( \frac{dV}{dV} \) is equal to the gradient \( \left( \frac{dy}{dx} \right) \) of the slope.

Where:

\( C = \text{capacitance} \)

\( e = \text{electron charge} \ (1.602 \times 10^{-19} \text{ C}) \)

\( \varepsilon_0 = \text{permittivity of vacuum} \ (8.854 \times 10^{-12} \text{ F m}^{-1}) \)

\( \varepsilon = \text{dielelectric constant of the GO} \ (\sim 1000 \ [3]). \)

\( V = \text{applied bias potential} \)

\( E_{FB} = \text{flat band potential} \)

\( k = \text{Boltzmann constant} \)

\( T = \text{temperature} \)

\( N_A = \text{acceptor/hole density} \)

Therefore,

\( \text{Gradient}_{G-0} = -1.52 \times 10^{11} \text{ F}^{-2} \text{ cm}^4 \text{ V}^{-1} \)

\( N_{A G-0} = 9.28 \times 10^{15} \text{ cm}^{-3} \)
\[ \text{Gradient}_{G-2} = -1.22 \times 10^{11} \text{ } F^{-2} \text{ } cm^4 V^{-1} \]

\[ N_{A_G-2} = 1.16 \times 10^{16} \text{ } cm^{-3} \]

**Eqn (S3).** Calculation of conduction band potential.

\[ E_{CB} = E_{VB} - E_{BG} \quad \text{(S3)} \]

Where,

\[ E_{CB} = \text{Conduction band potential (V)} \]

\[ E_{VB} = \text{Valence band potential (V)} \]

\[ E_{BG} = \text{Band gap energy (eV)} \]

Thus,

\[ E_{CB_{G-0}} = 2.23 - 3.75 = -1.52 \text{ } V \]

\[ E_{CB_{G-2}} = 2.17 - 3.10 = -0.93 \text{ } V \]

**References**
