Supplementary Information
of

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

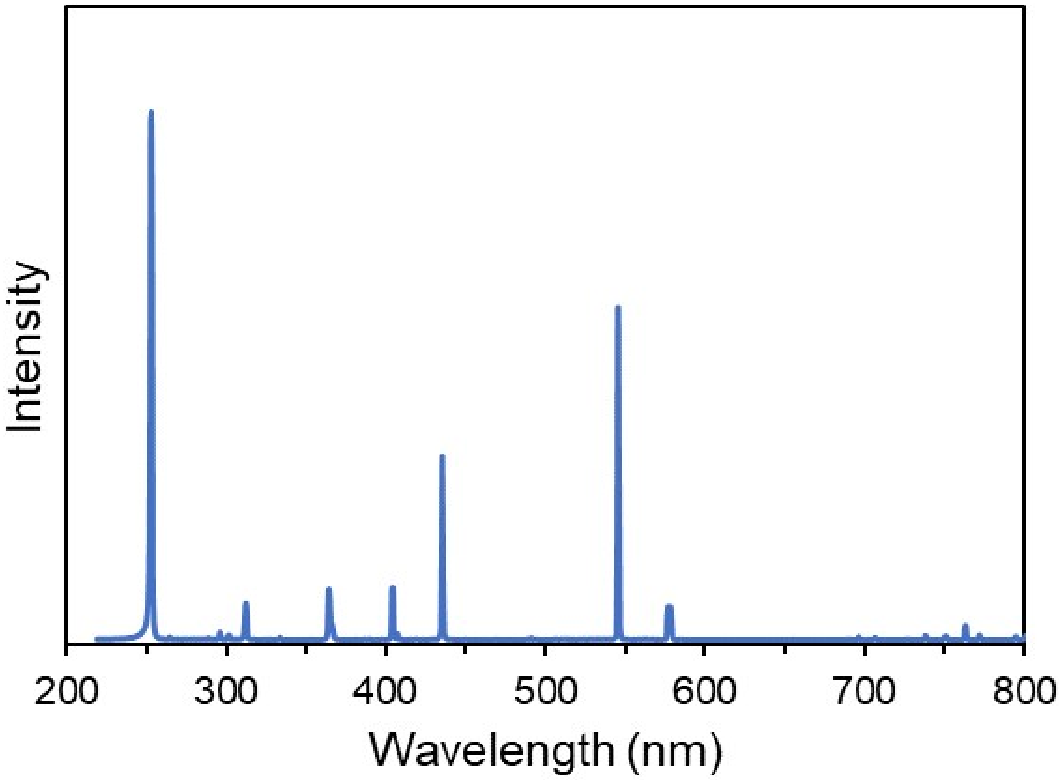

Fig. S1. Light spectrum of UV-C light source for photodegradation experiment.

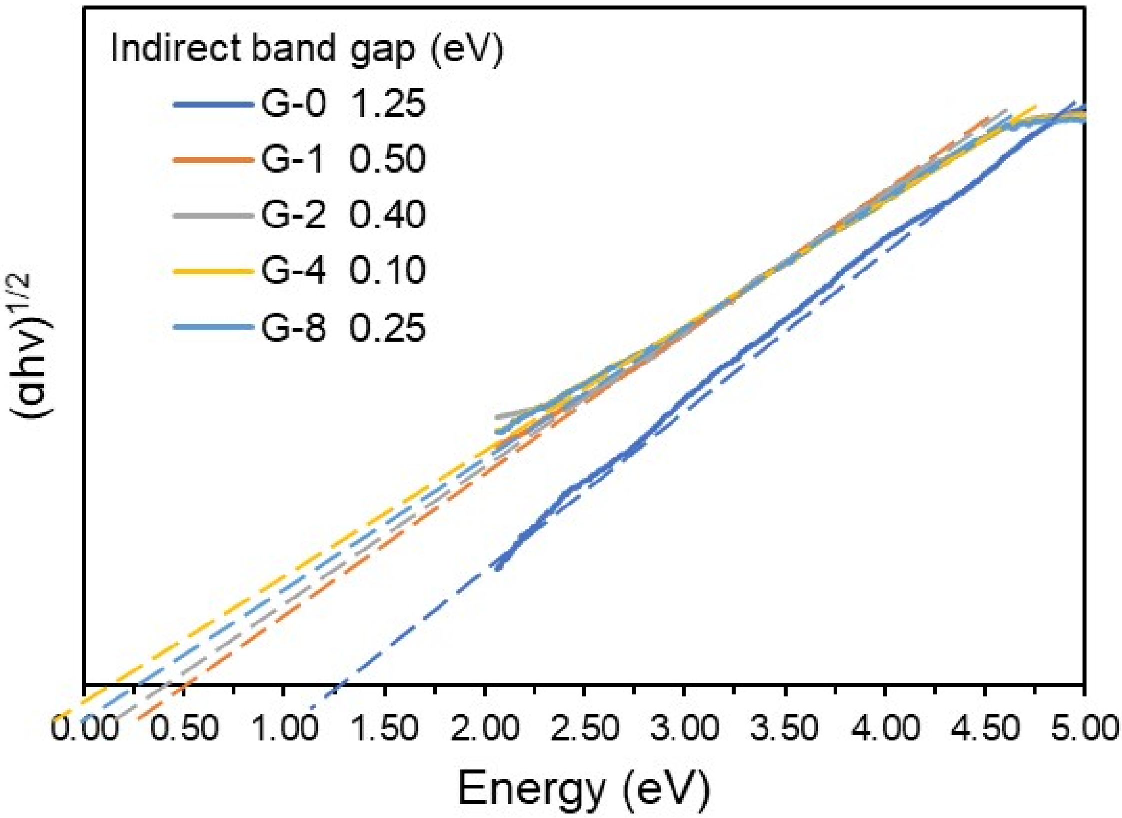

Fig. S2. Tauc plot for indirect band gap of G-0 to G-8.

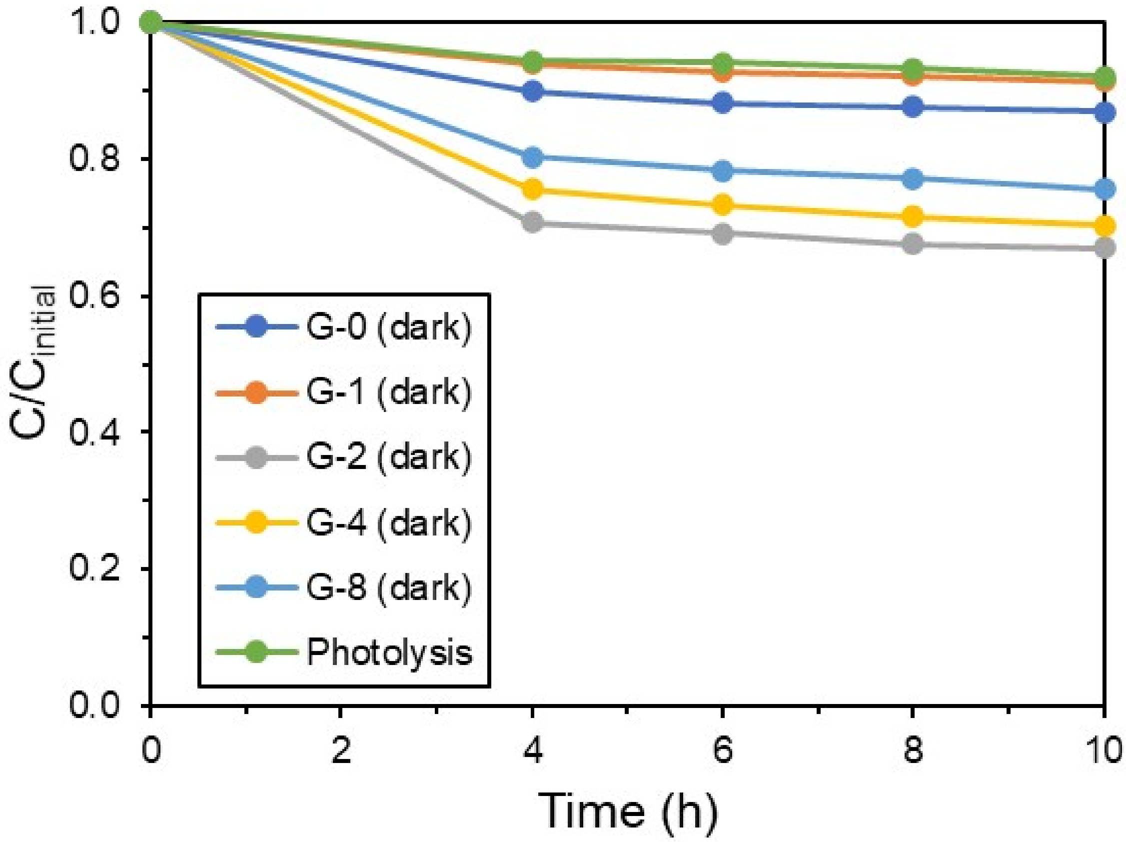

Fig. S3. 50 ppm MB for photolysis, and dark adsorption by G-0 to G-8.

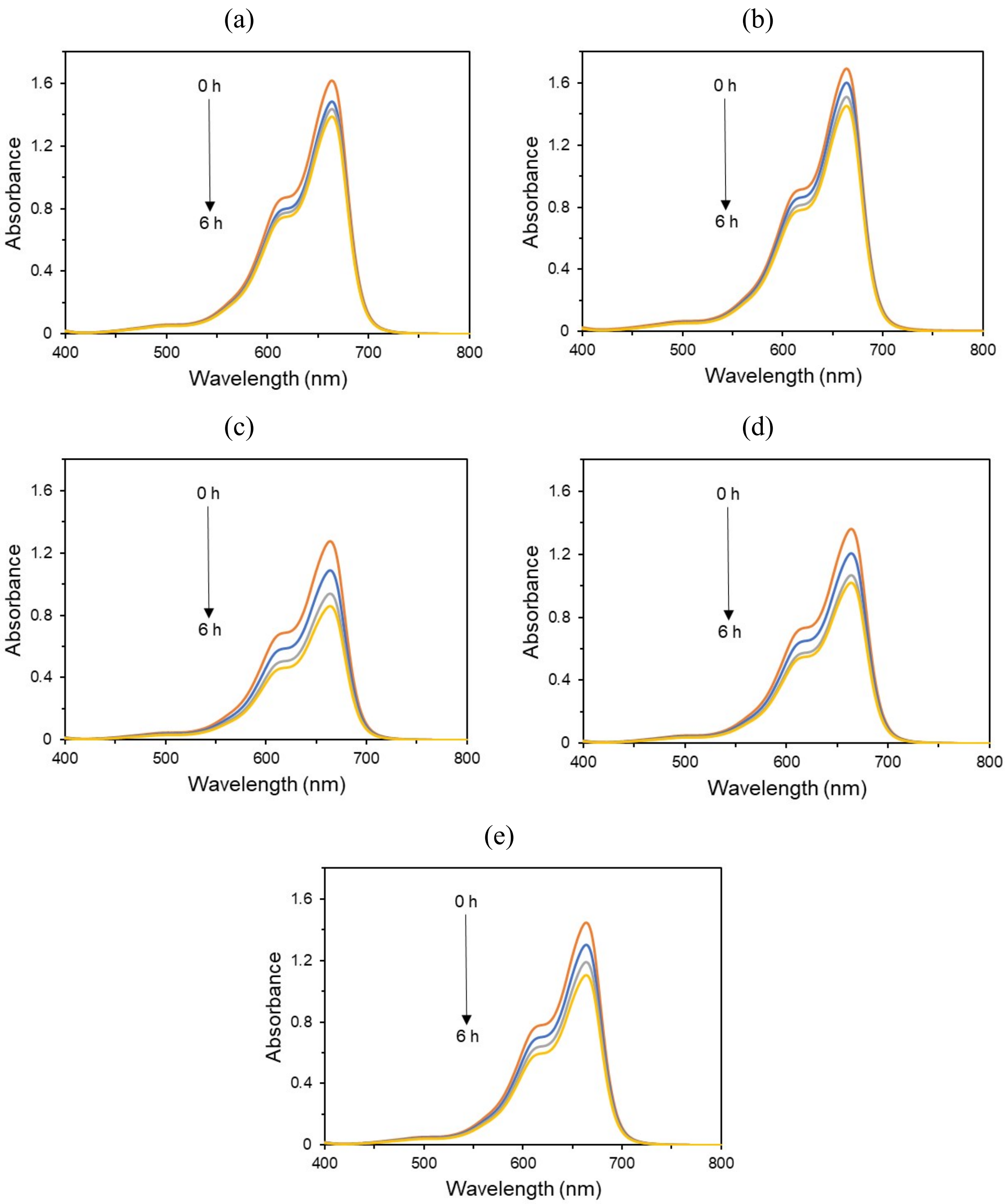

Fig. S4. Time-dependent UV-Vis absorption spectra for photodegradation of 50 ppm MB from time 0 to 6 h by (a) G-0, (b) G-1, (c) G-2, (d) G-4, and (e) G-8.

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

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

$$E_{NHE,\ pH\ 7} = E_{(Ag/AgCl\ pH\ 6.5)} + 0.21 - 0.059 \times (7.0 - 6.5) \tag{S1}$$

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

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

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

$$-\frac{\frac{1}{C^2}}{dV} = \frac{2}{e\varepsilon_0\varepsilon N_A} \qquad \text{(S2)}$$

$$-gradient = \frac{2}{e\varepsilon_0\varepsilon N_A}$$

$$N_A = -\frac{2}{e\varepsilon_0\varepsilon(gradient)}$$

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 $\frac{\frac{1}{C^2}}{dV}$ is equal to the gradient $\left(\frac{dy}{dx}\right)$ of the slope.

Where:

$C = capacitance$

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

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

$\varepsilon = dilectric\ constant\ of\ the\ GO$ (~1000 [3]).

$V = applied\ bias\ potential$

$E_{FB} = flat\ band\ potential$

$k = Boltzmann\ constant$

$T = temperature$

$N_A = acceptor/hole\ density$

Therefore,

$Grandient_{G-0} = -1.52 \times 10^{11}\,F^{-2}cm^4V^{-1}$

$N_{A_{G-0}} = 9.28 \times 10^{15}\,cm^{-3}$

$Grandient_{G-2} = -1.22 \times 10^{11}\ F^{-2}cm^{4}V^{-1}$

$N_{A_{G-2}} = 1.16 \times 10^{16}\ cm^{-3}$

Eqn (S3). Calculation of conduction band potential.

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

Where,

$E_{CB} = Conduction\ band\ potential\ (V)$

$E_{VB} = Valence\ band\ potential\ (V)$

$E_{BG} = Band\ gap\ energy\ (eV)$

Thus,

$E_{CB_{G-0}} = 2.23 - 3.75 = -1.52\ V$

$E_{CBG-2} = 2.17 - 3.10 = -0.93\ V$

References

1. Giannakopoulou, T., et al., *Tailoring the energy band gap and edges' potentials of g-C3N4/TiO2 composite photocatalysts for NOx removal.* Chemical Engineering Journal, 2017. **310**: p. 571-580.

2. Sahoo, P.P., B. Zoellner, and P.A. Maggard, *Optical, electronic, and photoelectrochemical properties of the p-type Cu 3− x VO 4 semiconductor.* Journal of Materials Chemistry A, 2015. **3**(8): p. 4501-4509.
3. Hong, X., W. Yu, and D. Chung, *Electric permittivity of reduced graphite oxide.* Carbon, 2017. **111**: p. 182-190.