

Supporting Information

Heterostructured TiO₂@OC Core@Shell Photocatalysts for Highly Efficient Waste Water Treatment

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Corresponding to the linear forms of equations 9 and 10 for the analysis of photodegradation kinetics, the more general non-linear 1st and 2nd order formulas are shown as equations S1 and S2:

Non-linear 1st order kinetic model:

$$q_t = q_e(1 - e^{-K_1 t}) \quad [S1]$$

Non-linear 2nd order kinetic model:

$$q_t = \frac{K_2(q_e)^{2t}}{1 + K_2 q_e t} \quad [S2]$$

At the meantime, the simplified equation for the first order rate kinetics is shown below:

$$\ln \frac{C_0}{C} = Kt \quad [S3]$$

Where C_0 (mol/L) represents the initial concentration of the contaminant without the addition of photocatalysts and C (mol/L) is the concentration of the solution at a given time.

For thermodynamic analysis, a series of equations that were crucial for the determination of the equilibrium constant, the Gibbs free energy, the enthalpy of the reaction and the entropy involved in the reaction.

Equilibrium constant:

$$K = \frac{C_o - C_E}{C_E} \quad [S4]$$

Gibbs free energy:

$$\Delta G = -RT \ln K \quad [S5]$$

Enthalpy:

$$\left(\frac{\partial \frac{1}{K}}{\partial \frac{1}{T}} \right) = -\frac{\Delta H}{R} \quad [S6]$$

Entropy:

$$\Delta S = -\left(\frac{\Delta G - \Delta H}{T} \right) \quad [S7]$$

In equation S4, K is the equilibrium constant, C_0 (mol/L) is the initial concentration of the MB before mixing with the photocatalytic samples, and C_E (mol/L) is the concentration at equilibrium. In equation S5, ΔG (kJ) is the Gibbs free energy, R (J/mol K) is the gas constant, T (K) is the temperature at which the experiments were performed, and $\ln K$ is the natural logarithm of the equilibrium constant of the photodegradation system. The variables used for equations S6 and S7 are the same as the ones found in equations S4 and S5, and the state variables ΔH (kJ) and ΔS (J/K) represent enthalpy and entropy, respectively.