Enhanced Sulfamerazine Removal via Adsorption–Photocatalysis Using Bi$_2$O$_3$–TiO$_2$/PAC Ternary Nanoparticles

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Supplementary Materials

**Figure S1.** Plot of $q$-$t$ for the adsorption of SMZ onto Bi$_2$O$_3$-TiO$_2$/PAC composites.

**Figure S2.** Adsorption isotherm of SMZ adsorption on Bi$_2$O$_3$-TiO$_2$/PAC with different calcination temperature.
Figure S3. Photocatalytic efficiencies, Bi$_2$O$_3$-TiO$_2$/PAC with different calcination temperature.

Figure S4. Photocatalytic efficiencies of Bi$_2$O$_3$-TiO$_2$/PAC with different calcination temperature.
**Figure S5.** Bi$_2$O$_3$-TiO$_2$/PAC(10%-700°C) microstructure image. FE-SEM image (a), SEM-EDS spectra (b), HRTEM micrograph (c) and the lattice parameters for composite (d).
Figure S6. TOC removal in the photodegradation of SMZ by Bi$_2$O$_3$-TiO$_2$/PAC(10%-700°C).
Table S1. Preparation method of Bi2O3-TiO2/PAC composites.

| Process                  | Steps                                                                 | Time (h) |
|--------------------------|----------------------------------------------------------------------|----------|
| Sol                      | (1) Sol (A): 10 mL of titanium butoxide slowly poured into 5 mL of acetic acid, and then it was poured into 40 mL of anhydrous ethanol. Sol (B): Bi(NO3)3·5H2O (1.113g, 1.391g or 1.669g) was dissolved into 80 mL of deionized water. Sol (C): Sol (B) was dripped into Sol (A). | 2        |
| Impregnation             | (2) 0.5 g PAC was added into Sol (C) while mixing by a magnetic mixer at 350 rmp. | 5        |
| Hydrothermal             | (3) Resulting sol was transferred into a Teflon container inside a stainless-steel autoclave reactor for hydrothermal treatment and then ground to powder. | 12       |
| Two-stage calcination    | (4) First-stage calcination was calcinated in a tubular furnace under 300 °C temperature in air atmosphere. Second stage calcination condition was calcinated in a tubular furnace under temperature of 500 °C, 600 °C or 700 °C in N2 atmosphere. | 2, 3     |
Table S2. Adsorption kinetic and isotherm models used for data analysis.

| Types              | Models                              | Equations                                | Parameters                                      |
|--------------------|-------------------------------------|------------------------------------------|-------------------------------------------------|
| Kinetics           | Pseudo first-order [30]             | \[ \log(q_e - q_t) = \log q_e - \frac{K_1}{2.303}t \] | \( K_1 \): pseudo first-order rate constant     |
|                    | Pseudo second-order [31]            | \[ \frac{t}{q_t} - \frac{t}{q_e} = \frac{1}{K_2q_e} \] | \( K_2 \): pseudo second-order rate constant    |
|                    | Intra-particle diffusion [32]       | \[ q_t = K_d t^{0.5} + C \]               | \( K_d \): intra-particle diffusion rate constant|
|                    | Boyd’s external diffusion [33]      | \[ q_t = q_{\infty}(1 - e^{-Rt}) \]       | \( R \): rate coefficient; \( q_{\infty} \): equilibrium adsorption capacity at infinite time |
|                    | Weber and Morris [34]               | \[ q_t = k_w t^{1/2} \]                   | \( k_w \): intraparticle diffusion coefficient  |
|                    | Langmuir kinetic [35]               | \[ \frac{dq_t}{dt} = k_a C_e (q_e - q_t) - k_d q_t \] | \( k_a \): adsorption rate constant; \( k_d \): desorption rate constant |
|                    | Langmuir [36]                       | \[ q_e = \frac{q_m K_L C_e}{1 + K_L C_e} \] | \( K_L \): Langmuir isotherm constant; \( q_m \): maximum adsorption capacity |
|                    | Freundlich [37]                     | \[ q_e = K_F C_e^{1/n} \]                 | \( K_F \): Freundlich isotherm constant; \( 1/n \): absorption capacity |

Table S3. Main water quality of surface water.

| Parameter           | Tonghui River | Lianshi Lake |
|---------------------|---------------|--------------|
| Temperature (°C)    | 18.5 ± 2.5    | 18.5 ± 2.5   |
| pH                  | 7.46 ± 0.3    | 7.11 ± 0.3   |
| Turbidity (NTU)     | 2.86 ± 0.52   | 1.73 ± 0.41  |
| DOC (mg L⁻¹)        | 2.406 ± 0.195 | 2.244 ± 0.104|
| UV254 (cm⁻¹)        | 0.109 ± 0.005 | 0.085 ± 0.007|

Table S4. Adsorption kinetic parameters of Bi₂O₃-TiO₂/PAC composites with different calcination temperatures.

| Composites                  | pseudo first-order | pseudo second-order | Intra-particle diffusion |
|-----------------------------|--------------------|---------------------|--------------------------|
|                             | \( k_1 \) (h⁻¹)   | \( q_{\infty} \) (mg g⁻¹) | \( R^2 \) | \( k_2 \) (mg g⁻¹ h⁻¹) | \( q_e \) (mg g⁻¹) | \( R^2 \) | \( K_d \) (mg g⁻¹ h⁻¹) | \( C \) | \( R^2 \) |
| Bi₂O₃-TiO₂/PAC (10%-500 °C) | 0.058              | 1.449               | 0.897                    | 0.038          | 5.171               | 0.996          | 0.462         | 1.364          | 0.728 |
| Bi₂O₃-TiO₂/PAC (10%-600 °C) | 0.065              | 1.586               | 0.911                    | 0.023          | 4.829               | 0.991          | 0.450         | 0.832          | 0.809 |
Table S5. Chemical formulas and main fragments (m/z) of intermediate products.

| ID | Chemical Formula | m/z  | Proposed Structure |
|----|------------------|------|--------------------|
| A  | C₁₀H₁₀N₄O₄S      | 214.9| ![Structure A](image1) |
| B  | C₁₁H₁₃N₄O₃S⁺     | 264.8| ![Structure B](image2) |
| C  | C₁₁H₁₀N₄O₄S      | 276.8| ![Structure C](image3) |
| D  | C₇H₉N₃O₂S        | 200.9| ![Structure D](image4) |
| E  | C₁₁H₁₂N₄        | 200.9| ![Structure E](image5) |