**-** **Supplementary Information-**

### Rapid adsorption of triclosan and p-chloro-m-xylenol by nitrogen doped magnetic porous carbon

Qiuxing Lia, Li Huangb, Paijin Zhub, Min Zhongb, c, Shuxia Xu\*b, c \*

*a College of Earth Science, Chengdu University of Technology, Chengdu, Sichuan 610059, China*

*b College of Ecology and Environment, Chengdu University of Technology, Chengdu, Sichuan 610059, China*

*c State Environmental Protection Key Laboratory of Synergetic Control and Joint Remediation for Soil & Water Pollution, Chengdu University of Technology, Chengdu 610059, China*

*c*

**1. Experimental Section  
1.1 Chemicals**

2-methylimidazole, Disodium hydrogen phosphate, Cobalt nitrate, P-chloro-m-xylenol (PCMX) and sodium hydroxide were purchased from Chengdu Kelong Chemical Reagent Factory. Triclosan (TCS) were supplied by Shanghai Macleans Biochemical Technology Company.Potassium Bromide were obtained from Shanghai Titan Technology Company. All chemicals were at least analytical grade and used as received. All aqueous solutions were prepared with ultra-pure water (18.25 mΩ·cm-1).

**1.2. Materials characterization**

**1.2.1 XRD Characterization of ZIF-67(Co) and Co-NPCs**

The crystal form of ZIF-67(Co) and Co-NPCs could be characterized by the multifunctional diffractometer (DX-2700BH, Dandong Haoyuan, China). kα ray of Cu target was used as ray source. The instrument tube voltage and current were 40 KV and 30 mA, respectively. The scan range of diffraction angle was 5-80o, and the acquisition step length was 0.08o.

**1.2.2 SEM Characterization of ZIF-67(Co) and Co-NPCs**

The morphology of ZIF-67(Co) and Co-NPCs were observed by the scanning electron microscope (HITACHI S-4800, Hitachi, Japan). In order to enhance the conductivity of the sample, the surface of the material was sprayed with gold. Moreover, the working distance and voltage were 9.6 mm and 10 kV, respectively.

**1.2.3 IR Characterization of ZIF-67(Co) and Co-NPCs**

The functional groups of ZIF-67(Co) and Co-NPCs could be characterized by Fourier Transform Infrared Spectrometer (Cary 630, Agilent, America). Before the test, a small amount of dried material and KBr were evenly mixed under an infrared baking lamp at a mass ratio of about 1:100, and then pressed into a tablet for spectral scanning. The scanning range was 400-4000 cm-1.

**1.2.4 XPS Characterization of Co-NPC-800**

In the experiment, the X-ray Photoelectron Spectrometer (ESCALAB 250Xi, Thermo Fisher, America) was used to analyze the element composition and valence state of ZIF-67(Co) and Co-NPC-800.

**1.2.5 Raman Spectroscopic Characterization of Co-NPC-800**

The Raman spectrum of Co-NPC-800 was tested with the confocal Raman microscope (HR-800, HORIBA JobinYvon, France). It was self-excited with Ar+, and the excitation wavelength was 514 nm.

**1.2.6 N2 isothermal adsorption-desorption curve test of Co-NPCs**

The N2 physical adsorption-desorption isotherms of Co-NPCs at 77K were measured by the automatic surface and porosity analyzer (ASAP 2460, Mike, America). Before the test, the sample was vacuum degassed at 300 oC for 3h. The specific surface area of the sample was calculated by the BET equation, and the pore diameter of the sample was calculated by the BJH model.

**1.3 Preparation of Co-NPCs suspension and pollutant stock solution**



**Figure S1.** **Working curve of (A) TCS or (C) PCMX;** **Absorption spectrum of (B) TCS or (D) PCMX.**

Preparation of Co-NPCs suspension: Transferred 25 mg of Co-NPC-800 sample to a 50 mL colorimetric tube, fixed the volume with ultrapure water, and 0.5 mg·mL-1 Co-NPC-800 suspension was obtained after ultrasonic for 1 h. Co-NPC-600, Co-NPC-700, Co-NPC-800(Ar) were also configured as suspensions of the same concentration under the same conditions.

Preparation of contaminant stock solution: Transferred 0.2 g of TCS and PCMX to a 100 mL volumetric flask respectively, fixed the volume with 1:1 ethanol and water, Then, TCS stock solution (200 mg·L-1) and PCMX stock solution (200 mg·L-1) were obtained after ultrasonic until the chemicals were completely dissolved. The stock solutions were stored in the refrigerator away from light and at low temperature for further use.

The absorbance of TCS and PCMX were measured by a UV-VIS Spectrometer (UV-5200PC, Shanghai Yuanxi Instrument Company), and the concentration of the two were calculated by Lambert Beer's law. The absorption spectra and working curves of TCS and PCMX were shown in **Figure S1**. It could be seen that the maximum absorption wavelength of both was around 280 nm. The working solution obtained by diluting the stock solution had a good correlation, conformed to Lambert Beer's law in a wide concentration range and could be used for quantitative calculation.

**1.4. Adsorption experiments of TCS and PCMX by Co-NPCs**

**1.4.1 The effect of pH on the adsorption performance of Co-NPC-800**

1 mL of PBS with different pH (pH=4, 5, 6, 7, 8, 9), 400 μL of Co-NPC-800 suspension, 200 μL of TCS stock solution and 400 μL ultrapure water (or 100 μL of PCMX stock solution and 500 μL ultrapure water) were added in a 2 mL centrifugal tube. The adsorption was carried out for 20 min in a 298 K water bath. Then, the supernatant was separated with a magnet. The concentrations of TCS/PCMX in the supernatant were analyzed by an UV−visible spectrophotometer at 280 nm. The amount of TCS/PCMX adsorbed on Co-NPC-800 in different pH were calculated from the expression E-1.

The Zeta potential of Co-NPC-800 at different pH were measured with the Nanoparticle Size and Potential Analyzer (ZEN 3600, Malvern, UK). The resistivity of Co-NPC-800 suspension was diluted to less than 1 Ω·cm during the measurement.

**1.4.2 The effect of NaCl concentration on the adsorption performance of Co-NPC-800**

1 mL of PBS (pH = 7.0) with different NaCl concentration (CNaCl = 0, 0.2, 0.4, 0.6, 0.8, 1.0 mol🞌L-1), 400 μL of Co-NPC-800 suspension, 200 μL of TCS stock solution and 400 μL ultrapure water (or 100 μL of PCMX stock solution and 500 μL ultrapure water) were added in a 2 mL centrifugal tube. The adsorption was carried out for 20 min in a 298 K water bath. Then, the supernatant was separated with a magnet. The concentrations of TCS/PCMX in the supernatant were analyzed by an UV−visible spectrophotometer at 280 nm. The amount of TCS/PCMX adsorbed on Co-NPC-800 in different NaCl concentration were calculated from the expression E-1.

**1.4.3 Adsorption kinetics**

1 mL of PBS (pH = 7.0), 400 μL of Co-NPC-800 suspension, 200 μL of TCS stock solution and 400 μL ultrapure water (or 100 μL of PCMX stock solution and 500 μL ultrapure water) were added into a 2 mL cuvette. Then placed the cuvette in the UV−visible spectrometer for kinetic scanning, and collected an absorbance at 280 nm every 5 s until the absorbance no longer changes.

**1.4.4 Adsorption Thermodynamics**

The TCS/PCMX solutions for adsorption thermodynamic experiments were prepared via serial dilution of the TCS/TCMX stock solution (200 mg·L-1) to desired concentrations with ultrapure water. 0.6 mL above solution of gradient concentration were added with 0.4 mL of Co-NPC-800 suspension and 1 mL of PBS (pH = 7.0) in several 2 mL centrifugal tube. The adsorption was carried out for 20 min in a 298 K, 308 K, 318 K water bath, respectively. Then, the supernatant was separated with a magnet. The concentrations of TCS/PCMX in the supernatant were analyzed by an UV−visible spectrophotometer at 280 nm. The amount of TCS/PCMX adsorbed on Co-NPC-800 in different temperature were calculated from the expression E-1.

**1.4.6 Practical application**

To remove insoluble impurities, the collected water samples were filtered with a 0.45 μm filter membrane. And the water samples were spiked to make the final concentration of TCS and PCMX be 20 and 10 mg·L-1 respectively. Afterward, repeated the adsorption procedures and calculated the adsorption capacity of Co-NPC-800 in actual water samples.



**Figure S2. XRD spectra of simulated ZIF-67 and synthesized ZIF-67.**



**Figure S3. SEM results of synthesized ZIF-67(Co) in different magnification, including (A) 10000×, (B) 50000×, (C) 100000×, and (D) 200000×.**



**Figure S4. Infrared spectra of synthesized ZIF-67(Co) and 2-methylimidazole.**



**Figure S5. XRD spectra of synthesized Co-NPC-800 and Co-NPC-800 (Ar).**



**Figure S6. Infrared spectra of synthesized Co-NPC-800 (Ar) and Co-NPC-800.**



**Figure S7. Raman spectra of synthesized Co-NPC-800.**



**Figure S8. XPS spectra of synthesized Co-NPC-800. (A) Full range, (B) N1s region with fitting and (C) Co2p region with fitting.**



**Figure S9. (A) N2 adsorption-desorption isotherms and (B) pore size distribution diagrams of Co-NPC-600, Co-NPC-800 and Co-NPC-800(Ar).**



**Figure S10. (A) Zeta potential of Co-NPC-800 at different pH values; (B) Zeta potential distribution of co-npc-800 at pH = 7.**



**Figure S11. The influence of NaCl concentration on the adsorption of (A) TCS or (B) PCMX by Co-NPC-800.**

**Table S1. The kinetic parameters of adsorption on Co-NPC-800 to TCS and PCMX**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Kinetic model | Quasi-first order dynamics model | | | Quasi-two-stage kinetic model | | |
| *q1e* (mg·g-1) | *k1* (min-1) | R2 | *q2e* (mg·g-1) | *k2* (g·mg-1·min-1) | *R2* |
| TCS | 37.003 | 0.311 | 0.958 | 143.678 | 0.02 | 0.994 |
| PCMX | 9.733 | 0.36 | 0.936 | 39.604 | 0.117 | 0.991 |

**Table S2. The isotherm model parameters of adsorption on Co-NPC-800 to TCS and PCMX**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Target | *T* (K) | Freundlich Model | | | Langmuir Model | | |
| *n* | *KF* | *R2* | *qm* | *KL* | *R2* |
| TCS | 298 | 3.776 | 73.127 | 0.883 | 163.132 | 0.596 | 0.999 |
| 308 | 3.781 | 102.569 | 0.923 | 219.78 | 0.679 | 0.993 |
| 308 | 3.935 | 108.44 | 0.902 | 262.467 | 0.728 | 0.994 |
| PCMX | 298 | 2.729 | 20.831 | 0.822 | 39.002 | 0.526 | 0.998 |
| 308 | 5.651 | 26.658 | 0.914 | 52 | 1 | 0.996 |
| 308 | 6.734 | 36.682 | 0.952 | 56.721 | 1.765 | 0.995 |

****

**Figure S12. Investigation on the reusability of Co-NPC-800 adsorbed (A) TCS and (B) PCMX**