

Supplementary Materials for

**Quantitative study of the enhanced content and chemical
stability of functional groups in mesoporous silica by in-situ co-
condensation synthesis**

Hao Zha^a, Tongxiao Zhou^a, Fengli Gan^a, Bangda Wang^{a, b}*, Zhongde Dai^{a, b}, Xia Jiang^{a, b}

^a College of Architecture and Environment, Sichuan University, Chengdu, 610065, China

^b National Engineering Research Center for Flue Gas Desulfurization, Chengdu, 610065, China

* Corresponding author. E-mail address: wang_bd@scu.edu.cn

Experimental S1: Study on demoulding efficiency of ethanol

The templating agent removal rate was studied by thermogravimetric analysis (TGA). Figure S1 showed the thermogravimetric diagram of raw material prepared by using P123 as the templating agent (untreated), and the same materials treated by calcination or ethanol to remove surfactant. The mass loss of the untreated material reached 46.3%, indicating that the residual content of templating agent was high in raw material. The calcined material had a low mass loss of less than 1%, demonstrating that the demolding process of the calcination method was thorough. The material treated with ethanol had a thermal weight loss of 4.5%. Although the demolding efficiency was slightly worse than the calcination method, most of the templating agent was removed compared with raw material, which showed that the ethanol method was also an effective method for the removal of surfactant in preparing functionalized mesoporous materials.

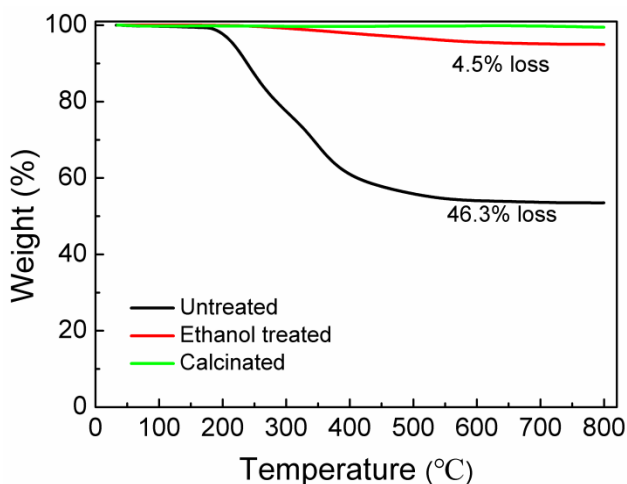


Figure S1. Thermal weight loss diagram of ethanol treated materials and calcine treated material. Treating process: calcining at 600°C for 4 hours and ethanol at 80°C for 8 hours.

Experimental S2. Pretreatment of wastewater.

In order to obtain a better purification effect, CaO pretreatment was applied to treat

the wastewater. As shown in Table S1, after 0.5 g/L of CaO treatment, the concentration of toxic metals in the wastewater decreased significantly. However, the solution after pretreatment fell short of emission standard due to the trace amount of toxic metals remained.

Table S1. Concentration of toxic metals (C_{0-p} , mg/L) before and after pretreatment.

| | | Pb | Cd | Ni | Cu | Zn | Mn |
|--------------------|-------|------|------|------|------|-------|------|
| Initial wastewater | C_0 | 21.1 | 49.4 | 95.6 | 79.8 | 243.8 | 17.4 |
| CaO pre-treated | C_p | 5.6 | 4.1 | 12.2 | 8.9 | 5.6 | 1.7 |

Experimental S3. Batch sorption experiments of sorbents for Pb (II).

The sorption capacity (q_t) and removal efficiency ($R\%$) were calculated from Equations.

(S1) and (S2).

$$q_t = \frac{(C_0 - C_t)V}{m} \quad (S1)$$

$$R(\%) = \frac{(C_0 - C_t)}{C_0} \times 100 \quad (S2)$$

Where C_0 and C_t are the Pb (II) concentrations of initial and at different process t , respectively; m is the sorbent mass; V is the solution volume.

In order to obtain the optimal sorbent dosage in the removal of Pb (II), the sorption capacities of sorbents (ami-MSN and MS denoted mesoporous silica with and without amino, respectively) with different dosage were studied. As shown in Figure S2, the removal efficiency of Pb (II) in the solution increased with the increase of sorbents dosage. When the dosage increased to 2g/L, the removal efficiency of Pb (II) in ami-MSN increased to 98.6%. With further increase of dosage, the removal efficiency of Pb (II) changed very slightly. The results showed that the optimal dosage of ami-MSN was

2g/L, with the removal efficiency of Pb (II) reaching 98.6%. It was noteworthy that, in order to study the sorption specificity of amino groups on Pb (II), the sorption property of Pb (II) on mesoporous silica without amino groups (MS) was conducted in this study for comparison. It can be seen from Fig.S2 that the removal efficiency of MS for Pb (II) was obviously lower than that of ami-MSN. Under the dosage of 2g/L, the removal efficiency of MS for Pb (II) was only 9.1%, which suggested that ami-MSN had an excellent removal efficiency toward Pb (II).

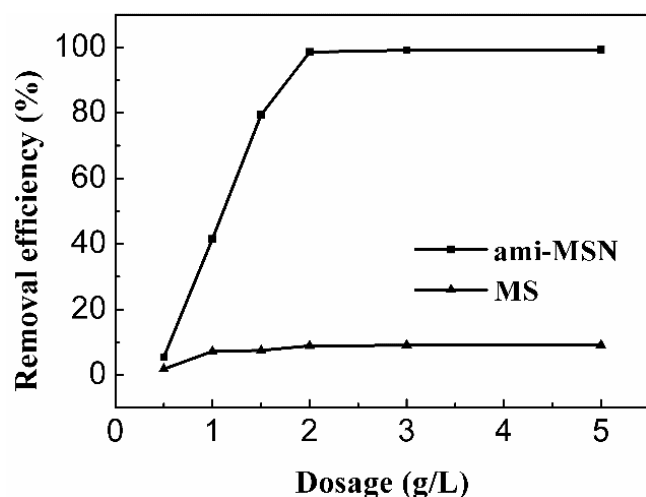


Figure S2. The removal efficiency of Pb (II) on ami-MSN and MS at different dosage. T = 30 °C and pH = 4. The concentration of Pb (II) is 500 ppm and the contact time is 4 h.

The Langmuir one-site equation (Equation S3) was applied to fit the experimental data [1,2]. The maximum adsorption capacity was predicted from sorption isotherms curve after reaching equilibrium (240 min).

$$q_e = \frac{b q_{max} C_e}{1 + b C_e} \quad (S3)$$

Where C_e is the concentration of Pb (II) in the solution after reaching sorption equilibrium; q_e is the sorption capacity of Pb (II) on the sorbent; q_{max} is the maximal sorption capacity; b is a constant relating to sorption process.

Figure S3 (a) showed the sorption kinetic curve of Pb (II) on ami-MSN. It can be seen that the sorption reached equilibrium at about 4 h, which indicated a fast sorption rate for Pb (II). This could be attributed to two aspects. First, under the sorption condition of pH = 5, ami-MSN showed electronegativity and had strong electrostatic attraction with Pb (II). The second was that ami-MSN had high specific surface area and order porous structure. A large number of amino functional groups distributed in the ami-MSN framework had strong binding ability with Pb (II), which made ami-MSN a fast sorption behavior for Pb (II). Figure S3 (b) was the sorption isotherms of Pb (II) on ami-MSN. As shown, the equilibrium sorption capacity of Pb (II) on ami-MSN reached 169.5 mg/g, and the sorption behavior was fitted perfectly with the typical Langmuir one-site adsorption model ($R^2 = 0.996$).

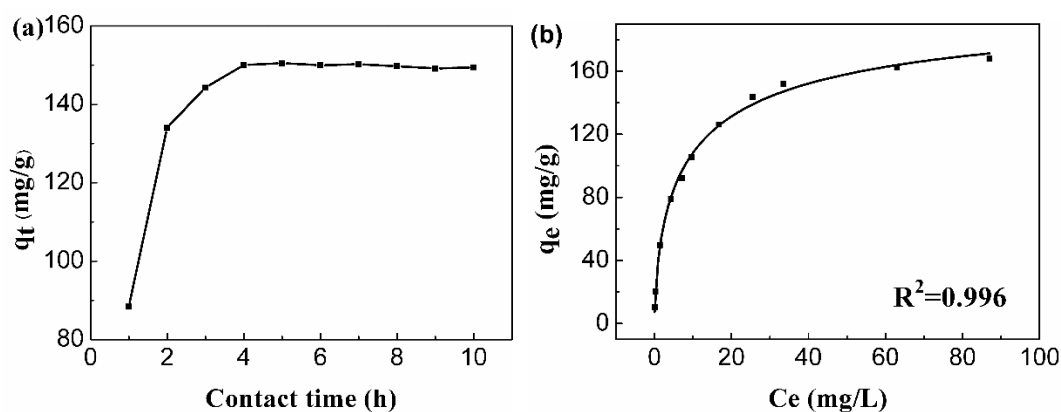


Figure S3. (a) Sorption kinetics of Pb (II) on ami-MSN. (b) Sorption isotherms of Pb (II) on ami-MSN, the symbols are experiment data, the line is the fitting curve using Langmuir one-site equation. Dosage of 2g/L at 30°C and pH=5.

Experimental S4. Determination of isoelectric point of ami-MSN.

The charging characteristics of the sorbent in the solution will affect its interaction with the target adsorbate. The pH of the solution will influence the surface potential of the sorbent and thus affect the sorption property. In order to avoid the interference of

electrostatic repulsion on the sorption properties between sorbents and target ions, the charge characteristics of ami-MSN in different pH environments were studied [3,4]. As the zeta potential versus pH curve for ami-MSN showed in Figure S3, the zero point of ami-MSN was at pH = 2.2 approximately, indicating that ami-MSN was negatively charged in an aqueous environment of pH higher than 2.2. For most positively charged heavy metal ions, ami-MSN showed electrostatic attraction with ions in the solution with pH higher than 2.2, which was benefit for improving the

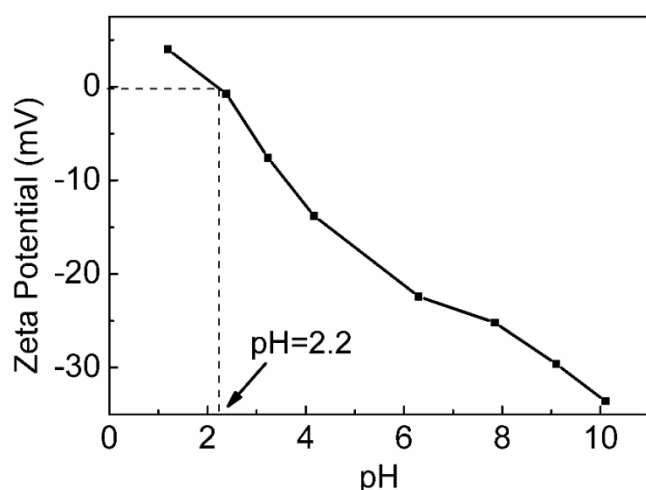


Figure S4. Zeta potential of ami-MSN as a function of pH.

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