Supporting Information

## Controllable synthesis of functionalized ordered mesoporous silica by metal-based ionic liquids, and their effective adsorption of dibenzothiophene

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Fig S1. TG of meso-Cu/SiO<sub>2</sub>(Cu-IL<sub>1</sub>) before thermal treatment.

The sample meso-Cu/SiO<sub>2</sub>(Cu-IL<sub>1</sub>) before thermal treatment was analyzed by thermo gravimetric (TG). This process was performed in N<sub>2</sub> atmosphere. As showed in Fig S1, the weight loss between room temperature and 100°C is only 1.39%, which due to the small amount of physisorbed water. It can be seen that there is a large weight loss of 43.36 % between 220 and 550°C. This is coursed by combustion and decomposition of the alkyl chains of imidazolium cation of ionic liquid. It can be found that there is no mass loss after 550°C, which indicated the organic part had been removed after 550°C.



Fig. S2. The FT-IR spectra of meso/SiO<sub>2</sub>(IL) and meso-Cu/SiO<sub>2</sub>(Cu-IL<sub>1</sub>)

Some others FT-IR bands were analyzed. The band at 1636 cm<sup>-1</sup> is the bending of the O-H.[1] The band at 1089 cm<sup>-1</sup> is the asymmetric stretch of Si-O-Si bonds. And the band at 458 cm<sup>-1</sup> is attributed to the Si-O bending vibration.[2] The result indicated that they are not related to some carbon-oxygen and / or carbon-nitrogen-based vibration modes.

[1] L. C. Fonseca, R. Faez, F. F. Camilo, M. A. Bizeto, *Micropor Mesopor Mater.*, 2012, 159, 24-29.

[2] X.C. Shao, X.T. Zhang, W.G. Yu, Y.Y. Wu, Y.C. Qin, Z.L. Sun, L.J. Song, *Appl. Surf. Sci.*, 2012, 263, 1-7.



Fig. S3. The low-angle XRD of meso-Cu/SiO<sub>2</sub>(Cu-IL<sub>2</sub>)



Fig. S4. The low-angle XRD of meso-Fe/SiO<sub>2</sub>(Fe-IL)



Fig. S5. The low-angle XRD of meso-Mn/SiO<sub>2</sub>(Mn-IL)



Fig. S6. The low-angle XRD of meso-Ni/SiO<sub>2</sub>(Ni-IL)



Fig. S7. The wide-angle XRD of meso-Cu/SiO<sub>2</sub>(Cu-IL<sub>2</sub>)



Fig. S8. The wide-angle XRD of meso-Fe/SiO<sub>2</sub>(Fe-IL)



Fig. S9. The wide-angle XRD of meso-Mn/SiO<sub>2</sub>(Mn-IL)



Fig. S10. The wide-angle XRD of meso-Ni/SiO<sub>2</sub>(Ni-IL)



Fig. S11.  $N_2$  adsorption-desorption isotherms and pore size distribution (the inset) of meso-Cu/SiO<sub>2</sub>(Cu-IL<sub>2</sub>)



Fig. S12.  $N_2$  adsorption-desorption isotherms and pore size distribution (the inset) of meso-Fe/SiO<sub>2</sub>(Fe-IL)



Fig. S13.  $N_2$  adsorption-desorption isotherms and pore size distribution (the inset) of meso-Mn/SiO<sub>2</sub>(Mn-IL)



Fig. S14.  $N_2$  adsorption-desorption isotherms and pore size distribution (the inset) of meso-Ni/SiO<sub>2</sub>(Ni-IL)



Fig. S15. XPS spectrum of meso-Cu/SiO<sub>2</sub>(Cu-IL<sub>1</sub>)

The survey XPS spectrum shows that the main elements on the surface of the product are Cu, O, Si and C. The C came from the adventitious carbon to correct for specimen. No N element was found, which implied the imidazolium cation of ionic liquid has been removed.



Fig.S16. XPS measurement for Si 2s level of meso-Cu/SiO<sub>2</sub>(Cu-IL<sub>1</sub>).



Fig. S17. Adsorption isotherms of DBT at 25°C on meso-Cu/SiO<sub>2</sub>(Cu-IL<sub>1</sub>)



Fig. S18. The FT-IR spectra of meso-Cu/SiO<sub>2</sub>(Cu-IL<sub>2</sub>)



Fig. S19. The FT-IR spectra of meso-Fe/SiO<sub>2</sub>(Fe-IL)



Fig. S20. The FT-IR spectra of meso-Mn/SiO<sub>2</sub>(Mn-IL)



Fig. S21. The FT-IR spectra of meso-Ni/SiO<sub>2</sub>(Ni-IL)

Table S1 The elemental	compositions of different samples
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Sample	N (%) <sup>a</sup>	C (%) <sup>a</sup>	Metal/Si (%) <sup>b</sup>
meso-Cu/SiO <sub>2</sub> (Cu-IL <sub>1</sub> )	0	0.33	1.44×10 <sup>-2</sup>
meso-Cu/SiO <sub>2</sub> (Cu-IL <sub>2</sub> )	0	0.077	6.94×10 <sup>-3</sup>
meso-Fe/SiO <sub>2</sub> (Fe-IL)	0	0.041	1.14×10 <sup>-2</sup>
meso-Mn/SiO <sub>2</sub> (Mn-IL)	0	0	3.85×10-3
meso-Ni/SiO <sub>2</sub> (Ni-IL)	0	0.089	1.02×10-3
meso-SiO <sub>2</sub> (IL)	0	0.33	-

<sup>a</sup> the data obtained by Elemental analysis, <sup>b</sup> obtained by ICP.

From the Table, it can be seen that the samples did not contain N elemental and hardly contained C elemental. So it can be concluded that the imidazolium rings were completely removed and the residual carbon was not present.

Sample	2-Theta			
	(100)	(110)	(200)	
meso-Cu/SiO <sub>2</sub> (Cu-IL <sub>1</sub> )	2.6	4.4	5.1	
meso-Cu/SiO <sub>2</sub> (Cu-IL <sub>2</sub> )	2.5	4.2	4.8	
meso-Fe/SiO <sub>2</sub> (Fe-IL)	2.5	4.3	5.0	
meso-Mn/SiO <sub>2</sub> (Mn-IL)	2.6	4.4	5.1	
meso-Ni/SiO <sub>2</sub> (Ni-IL)	2.8	4.7	5.4	

Table S2 The 2-Theta values and the (hkl) reflection lines for each sample