

# **One-pot synthesis of ordered mesoporous silica encapsulated polyoxometalates-based ionic liquids induced efficient desulfurization of organosulfur in fuel**

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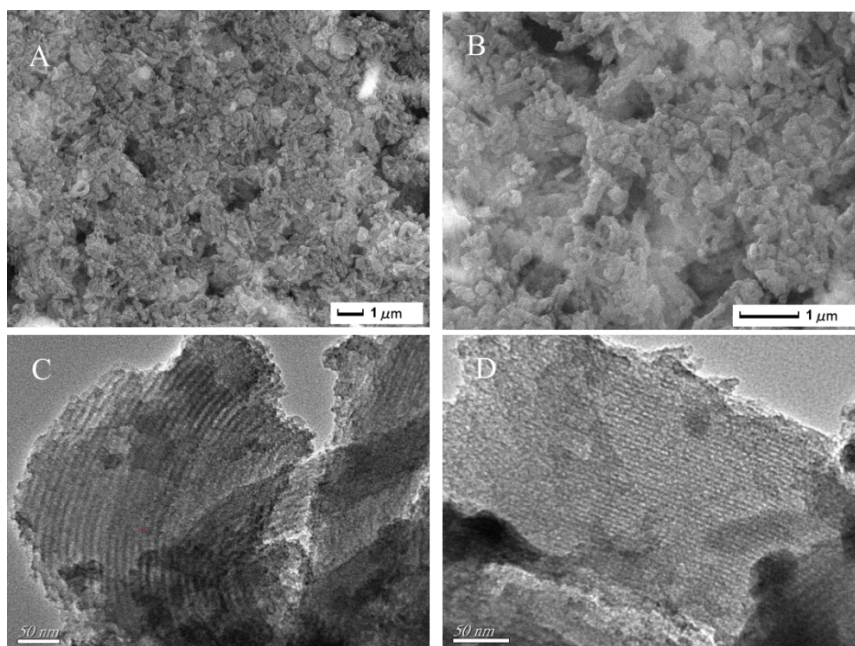
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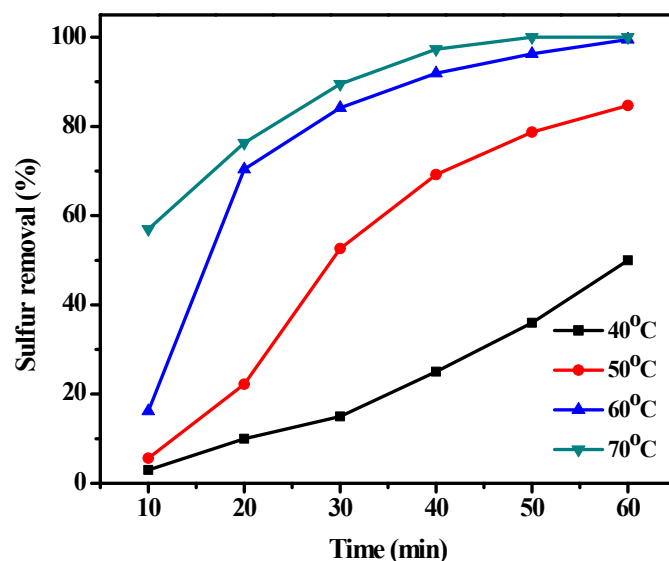
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**Fig. S1** SEM images of (A) C<sub>8</sub>-IL@OMS and (B) C<sub>16</sub>-IL@OMS; TEM images of (C) C<sub>8</sub>-IL@OMS and (D) C<sub>16</sub>-IL@OMS.

### **Influence of reaction temperature and time on the catalytic activity**

The catalytic activity of the heterogeneous catalyst was significantly influenced by the reaction temperature and time. As shown in Fig. S2, the desulfurization performance of as-synthesized was highly efficient on the removal of DBT with the reaction temperature increased. The sulfur removal could achieve 99.5% in 60 min at 60°C. However, the catalytic activity at 40 °C was only 50%, demonstrating that the reaction rate was limited by kinetics. In addition, when the reaction temperature was up to 70°C, the improvement of activity was not obvious in 60 min, which was attributed to the decomposition of H<sub>2</sub>O<sub>2</sub> with reaction temperature increased. From the aspects of economic consideration, the desulfurization system was tested in 60°C.

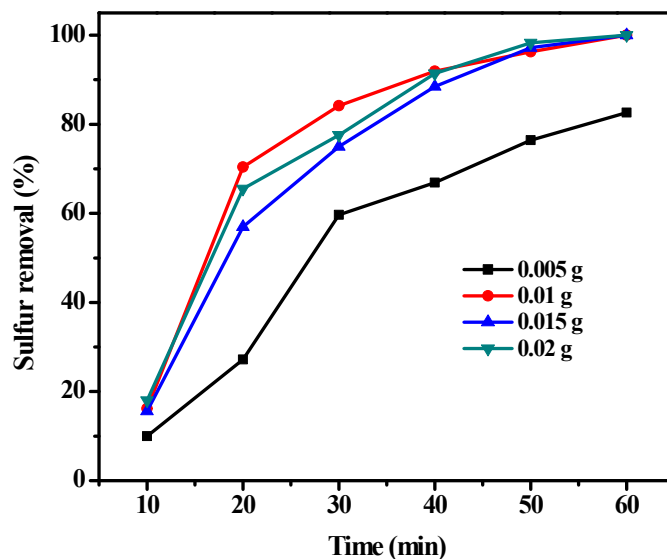


**Fig. S2** Influence of reaction temperature and time on the catalytic activity.

Reaction condition:  $m$  (catalyst) = 0.01 g, O/S = 3.

### **Influence of the amount of catalyst on the sulfur removal**

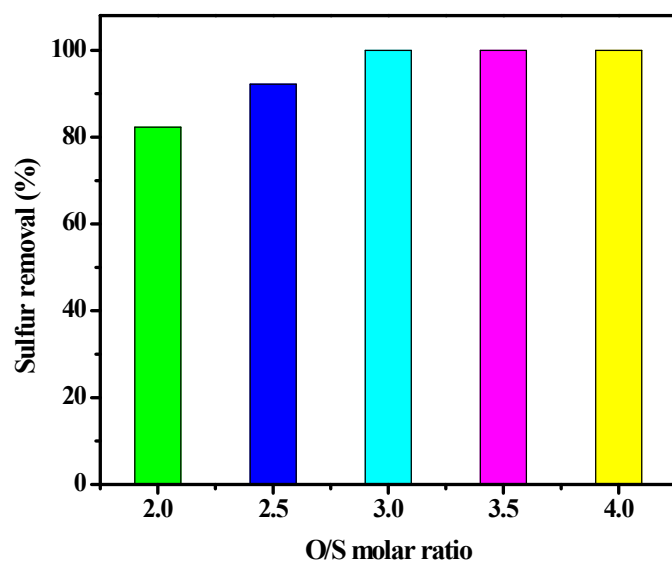
Fig. S3 exhibits the effect of the amount of as-prepared catalyst on the sulfur removal. It was distinctly observed that the conversion of DBT increased from 83% to 99.5% in 60 min by adjusting the amount of catalyst from 0.005 to 0.01 g. The results implied that less active species obtained could not achieve deep desulfurization. By increasing the amount of catalyst, more active sites were provided, leading to the obvious improvement of activity. However, it was worthy pointed out that the further increase of the mass of catalyst above 0.01 g, resulting in no rapidly promoted activity, which might be due to the aggregation of excessive catalyst in the presence of  $H_2O_2$ . Hence, it is not beneficial for the removal of DBT in the desulfurization process.



**Fig. S3** Influence of the amount of catalyst on the sulfur removal. Reaction condition: T = 60°C, t = 60 min, O/S = 3.

#### **Influence of O/S molar ratio on the catalytic activity**

The effect of O/S on the sulfur removal is depicted in Fig. S4. The removal of DBT could reach 82% when the molar ratio of H<sub>2</sub>O<sub>2</sub> was stoichiometric requirement (O/S= 2), indicating that partial oxidant decomposed during reaction. Excessive oxidant is helpful for removing sulfur-containing compounds in model oil. When the O/S increased to 3, 99.5% of DBT was oxidized to its corresponding sulfone. Further increasing the dosage of O/S from, the catalytic activity of C<sub>4</sub>-IL@OMS was not obviously improved, and the value of O/S = 3 was chosen as the optimal ratio in the subsequent examination.



**Fig. S4** Influence of O/S molar ratio on the catalytic activity of catalyst.

Reaction conditions:  $m(\text{C}_4\text{-IL@OMS}) = 0.01 \text{ g}$ ,  $T = 60^\circ\text{C}$ ,  $t = 60 \text{ min}$ .