

Molybdenum-containing dendritic mesoporous silica spheres for fast oxidative desulfurization in fuel

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Table S1. The theoretical and actual molybdenum contents in the hybrid materials.

Entry	Sample	Theoretical value (wt%)	Actual value ^a (wt%)
1	Mo/5SiO ₂ -550	24.2	16.1
2	Mo/10SiO ₂ -550	13.8	8.6
3	Mo/20SiO ₂ -550	7.4	4.1
4	Mo/10SiO ₂ -450	13.8	7.5
5	Mo/10SiO ₂ -650	13.8	6.9

^a Molybdenum content measured from ICP-OES.

The influence of reaction temperature on ODS activity is studied (Fig. S1). It is found that the sulfur removal was improved with the increase of the reaction temperature. The 4,6-DMDBT can be completely removed at 60 °C within 40 min. When the temperature rose to 70 °C, the time for the complete removal of 4,6-DMDBT was just reduced from 40 to 30 min. As the temperature reduced to 50 °C, the sulfur removal was only 85% within 60 min. The above results indicated that the reaction temperature was an important factor in ODS process. In view of economic point, 60 °C in 40 min was chosen as the optimal condition for the desulfurization process.

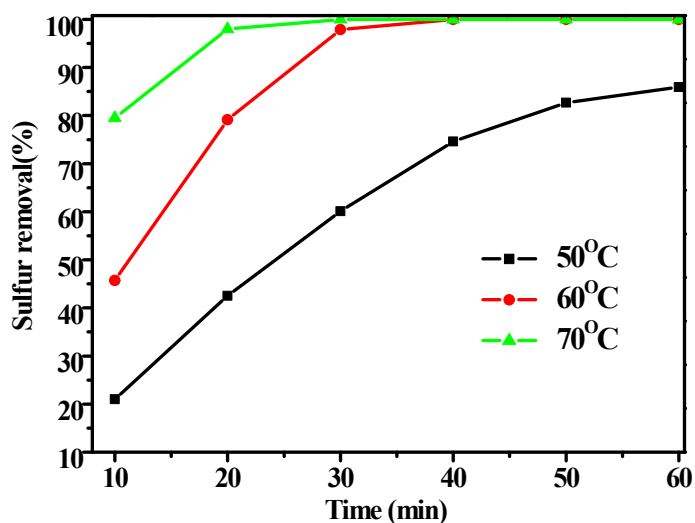


Fig. S1 Effect of reaction temperature on the removal of 4,6-DMDBT.

Reaction conditions: $m(\text{catalyst}) = 0.01 \text{ g}$, $O/S = 3$.

In order to investigate the influence of the oxidant dosage on the ODS process, the sulfur removal of 4,6-DMDBT with different TBHP/4,6-DMDBT molar ratios (Denoted as O/S) is examined (Fig. S2). It is obviously found that the increase of O/S has a positive effect on the oxidative desulfurization of 4,6-DMDBT. With $O/S = 1.5$, the sulfur removal could reach 85% in 60 min. When $O/S = 2$, the sulfur removal could reach 100% in 50 min. Furthermore, the sulfur compounds could be completely removed in 40 min with $O/S = 3$. Hence TBHP/4,6-DMDBT molar ratios = 3 was chosen as another optimal condition.

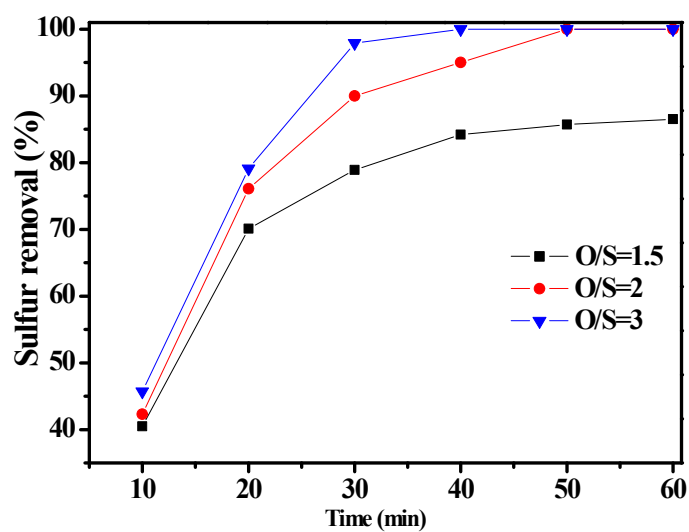


Fig. S2 Effect of the TBHP/4,6-DMDBT molar ratio (O/S) on sulfur removal.

Reaction conditions: $m(\text{catalyst})=0.01$ g, $T=60^{\circ}\text{C}$, $t=40$ min.

Fig. S3 displays the effect of the catalyst amount on the removal of 4,6-DMDBT. With low catalyst amount (0.005 g), the sulfur removal could only reach 73.1% in 40 min. When the catalyst amount was increased to 0.01 g, the sulfur compounds can be completely removed in 40 min. However, for the catalyst amount (0.02 g), the improvement in ODS activity is not clear. Taking the factors above into consideration, the catalyst amount was selected as 0.01g.

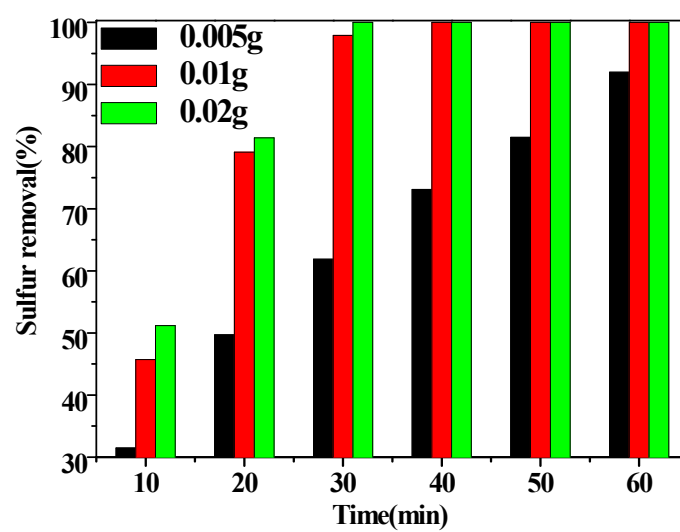


Fig. S3 Effect of the amount of the catalyst on sulfur removal. Reaction conditions:

O/S=3, T= 60°C, t= 40 min.