Supporting Information

Size-matched polyoxometalate encapsulated in UiO-66(Zr): an extraordinary catalyst with double active sites for highly efficient ultra-deep oxidative desulfurization of fuel oil

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Experimental

Preparation of Mo₈

1.25 g Na₂MoO₄·2H₂O was dissolved in 3 ml water, adjust the solution pH to 4.5 with HCl (1.0 ml, 6 mol/l), then add 0.80 g (n-C₄H₉)₄NCl, filter out the resulting precipitation, finally wash the precipitation thoroughly with water, absolute ethyl alcohol, acetone, diethyl ether, respectively.

Characterization

Figure S1. FE-SEM images of UiO-66 (a), Mo₈-UiO-66 (b).

Figure S2. EDS analysis of Mo₈-UiO-66.
Figure S3. TEM images of Mo₈-UiO-66 (a) and element mapping (b).

Figure S4. Nitrogen adsorption-desorption isotherms of UiO-66 and Mo₈-UiO-66.
Figure S5. Aperture distribution of UiO-66 and Mo$_8$-UiO-66.

Figure S6. Thermogravimetric analysis of UiO-66 and Mo$_8$-UiO-66.

Figure S7. Reaction kinetics of DBT removal, reaction conditions: 60 °C, O/S = 4, $m_{\text{cat}} = 0.020$ g, t = 10 min.
Figure S8. PXRD patterns of Mo$_8$-UiO-66 and Mo$_8$-UiO-66 after fourth recycle.

Figure S9. FT-IR spectra of Mo$_8$-UiO-66 and Mo$_8$-UiO-66 after fourth recycle.
Figure S10. GC-MS of fresh model oil phase (a), oil phase after reaction (b), oxidative production after reextraction (c).

Figure S11. EPR spectrum of Mo$_8$-UiO-66, H$_2$O$_2$ and DMPO.

Table S1. The content of Mo$_8$ in different conditions (measured by ICP).

<table>
<thead>
<tr>
<th>Samples</th>
<th>Content of Mo$_8$</th>
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<tbody>
<tr>
<td>Mo$_8$-UiO-66</td>
<td>28.05%</td>
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<tr>
<td>Mo$_8$-UiO-66 (after reaction)</td>
<td>27.88%</td>
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