Electronic Supplementary Information

Deep oxidative desulfurization of dibenzothiophene with \( \text{Mo}_{132} \) nanoball supported on activated carbon as efficient catalyst at room temperature

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Fig. S1. UV-Vis spectrum of \{\text{Mo}_{132}\} aqueous solution

Fig. S2. TEM images of prepared \{\text{Mo}_{132}\} in ethanol
Fig. S3. Nitrogen adsorption/desorption isotherms of $\{\text{Mo}_{132}\}$
H$_2$-TPR analysis:

The H$_2$-temperature programmed reduction (H$_2$-TPR) experiment was performed on 50 mg of the catalyst (\{Mo$_{132}$\}/AC-20) placed in a U-shaped quartz reactor. Prior to the TPR run, the catalyst was degassed in flow of 10 sccm Ar at 110°C for 1 hour, and cooled down to 40°C. Then, the sample was heated from 40 to 900°C at a heating rate of 10°C/min in a flow of 5% H$_2$/Ar mixture (10 sccm).

The H$_2$-TPR was employed to study the reducibility of the catalyst. As shown in Fig. S4, \{Mo$_{132}$\}/AC-20 exhibited two reduction peaks, a sharp peak at 560°C and a weak peak at higher temperature of 710 °C. These two peaks indicate reduction of Mo$^{VI}$ and Mo$^{VI}$ in \{Mo$_{132}$\} cluster in the catalyst.

![Fig. S4. H$_2$-TPR profile of \{Mo$_{132}$\}/AC-20](image-url)
Table S1
Reusability of {Mo₁₃₂}/AC-20 and {Mo₁₃₂} content of the catalyst in each step

<table>
<thead>
<tr>
<th>Catalyst samples</th>
<th>DBT removal (%)</th>
<th>Actual {Mo₁₃₂} contents (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fresh catalyst</td>
<td>99.5</td>
<td>9.04</td>
</tr>
<tr>
<td>1&lt;sup&gt;st&lt;/sup&gt; reuse</td>
<td>98.1</td>
<td>8.59</td>
</tr>
<tr>
<td>2&lt;sup&gt;nd&lt;/sup&gt; reuse</td>
<td>97.8</td>
<td>8.38</td>
</tr>
<tr>
<td>3&lt;sup&gt;rd&lt;/sup&gt; reuse</td>
<td>97.7</td>
<td>8.35</td>
</tr>
</tbody>
</table>
Dibenzothiophene sulfone
Fig. S5. GC-MS analysis of the acetonitrile phase at the end of the process. (a) GC-MS chromatogram, (b) The standard mass spectrum of DBT sulfone, (c) The mass spectrum of the oxidation product of DBT. Reaction condition: T = 25 °C, {Mo$_{132}$/AC-20 catalyst dosage = 0.0025 g cat/ g F, O/S = 10, t = 30 min, initial sulfur content = 500 ppm.