

## 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

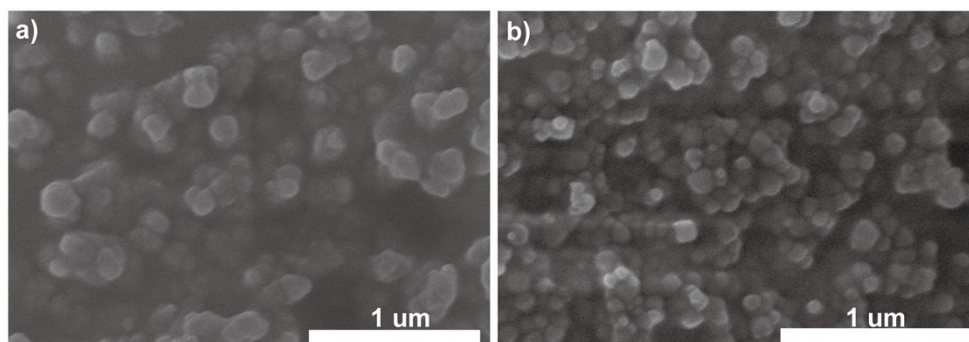
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#### Experimental

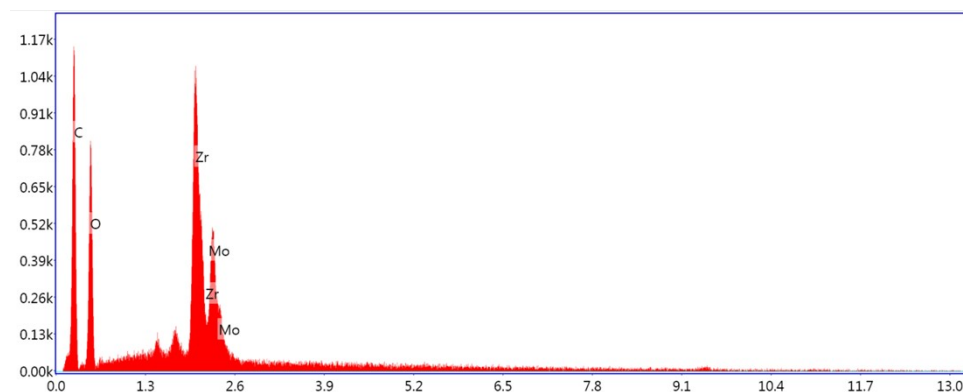
##### Preparation of $\text{Mo}_8$

1.25 g  $\text{Na}_2\text{MoO}_4 \cdot 2\text{H}_2\text{O}$  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  $(n\text{-C}_4\text{H}_9)_4\text{NCl}$ , filter out the resulting precipitation, finally wash the precipitation thoroughly with water, absolute ethyl alcohol, acetone, diethyl ether, respectively.

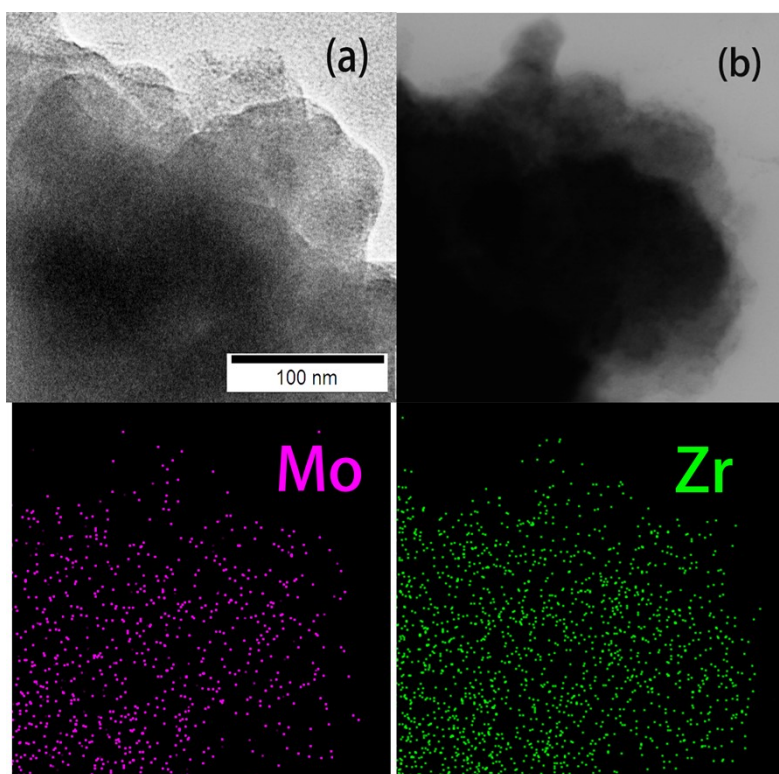
#### Characterization



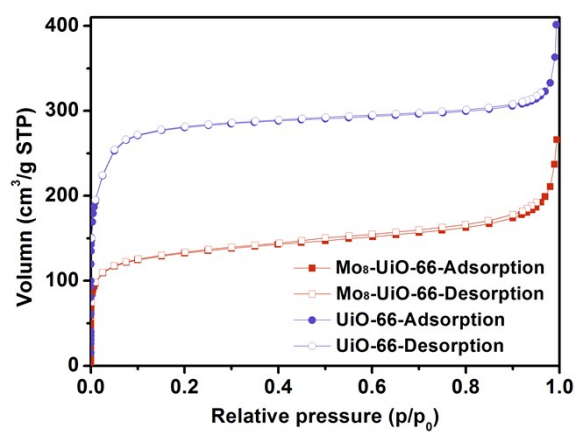
**Figure S1.** FE-SEM images of UiO-66 (a),  $\text{Mo}_8$ -UiO-66 (b).



**Figure S2.** EDS analysis of  $\text{Mo}_8$ -UiO-66.



**Figure S3.** TEM images of Mo<sub>8</sub>-UiO-66 (a) and element mapping (b).



**Figure S4.** Nitrogen adsorption-desorption isotherms of UiO-66 and Mo<sub>8</sub>-UiO-66.

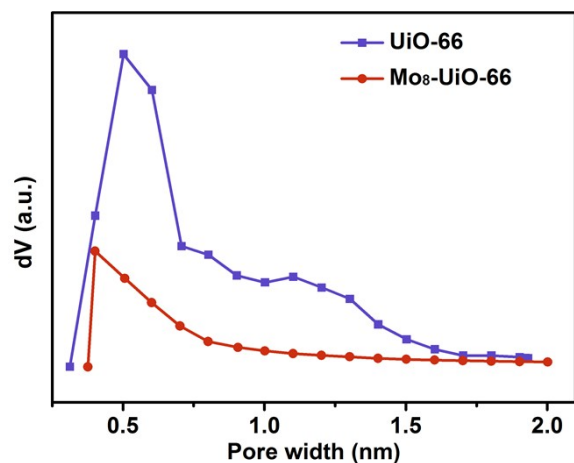


Figure S5. Aperture distribution of UiO-66 and Mo<sub>8</sub>-UiO-66.

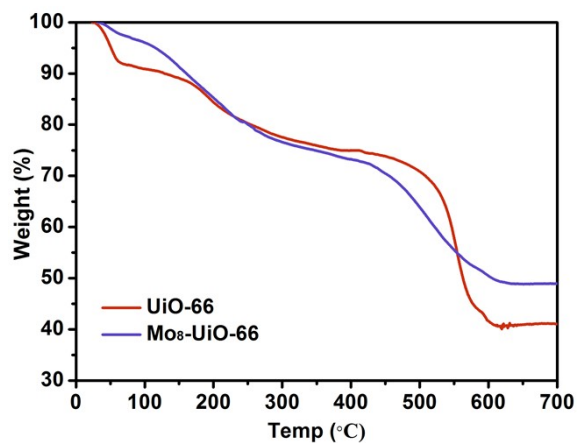


Figure S6. Thermogravimetric analysis of UiO-66 and Mo<sub>8</sub>-UiO-66.

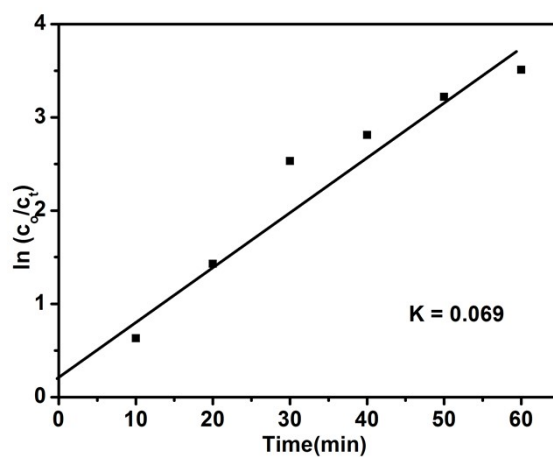
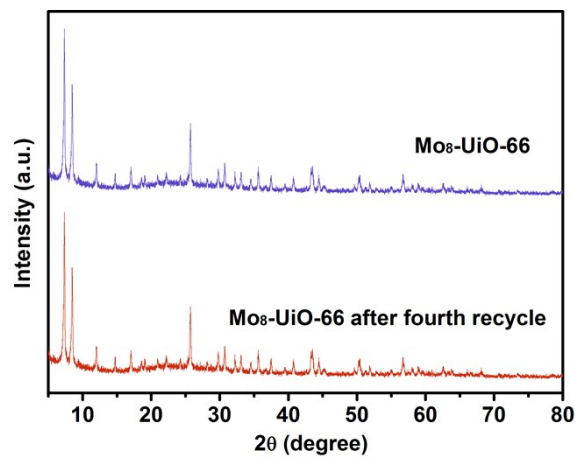
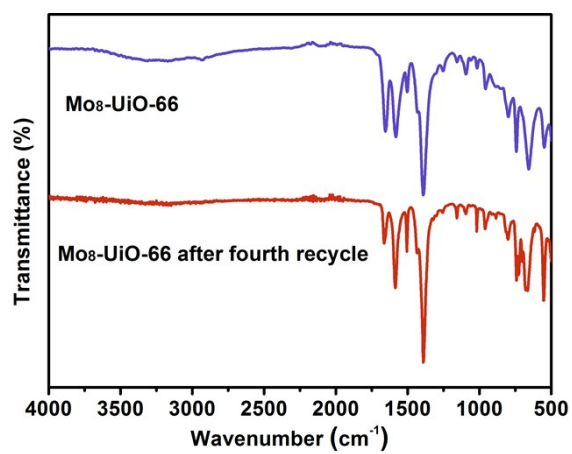


Figure S7. Reaction kinetics of DBT removal, reaction conditions: 60 °C, O/S = 4,  $m_{\text{cat}} = 0.020$  g,  $t = 10$

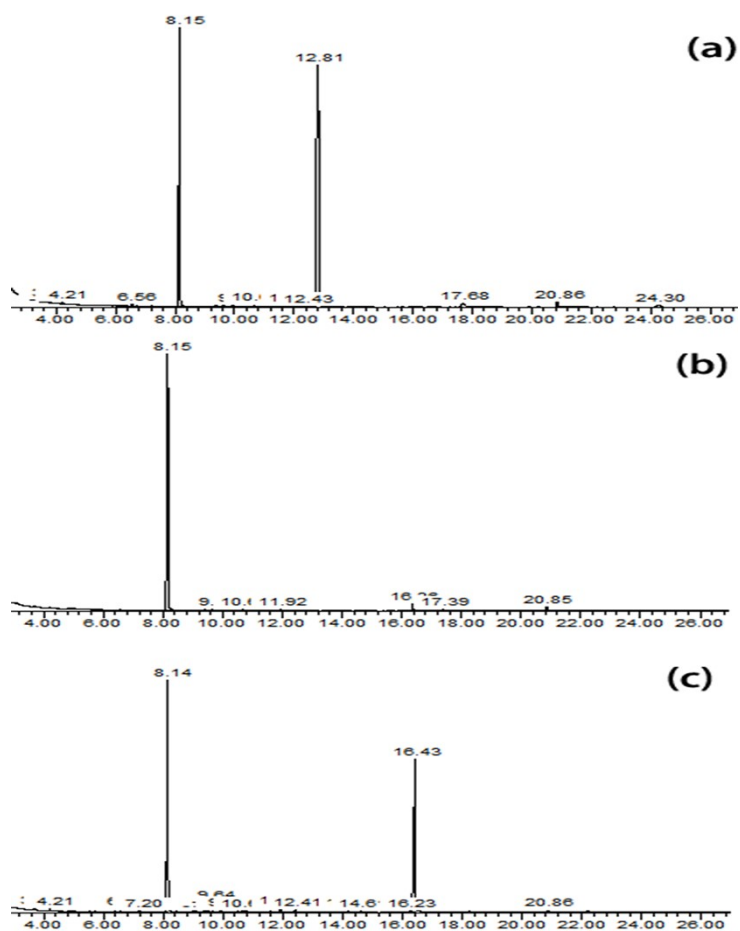
min.



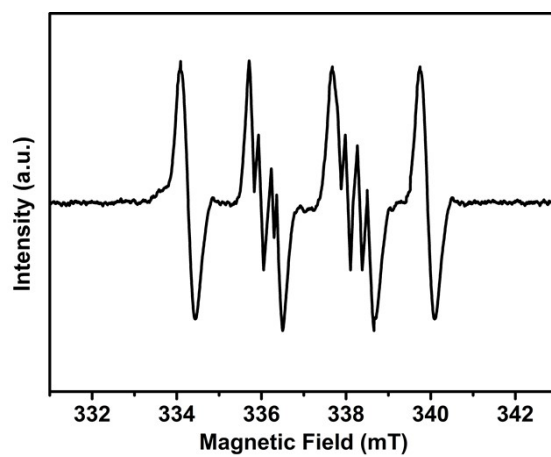
**Figure S8.** PXRD patterns of Mo<sub>8</sub>-UiO-66 and Mo<sub>8</sub>-UiO-66 after fourth recycle.



**Figure S9.** FT-IR spectra of Mo<sub>8</sub>-UiO-66 and Mo<sub>8</sub>-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  $\text{Mo}_8\text{-UiO-66}$ ,  $\text{H}_2\text{O}_2$  and DMPO.

**Table S1.** The content of  $\text{Mo}_8$  in different conditions (measured by ICP).

Samples	Content of $\text{Mo}_8$
$\text{Mo}_8\text{-UiO-66}$	28.05%
$\text{Mo}_8\text{-UiO-66}$ (after reaction)	27.88%