

# Supplementary Information of

## **A novel MOF-808 derived material for oxidative desulfurization: the synergistic effect of hydrophobicity and electron transfer**

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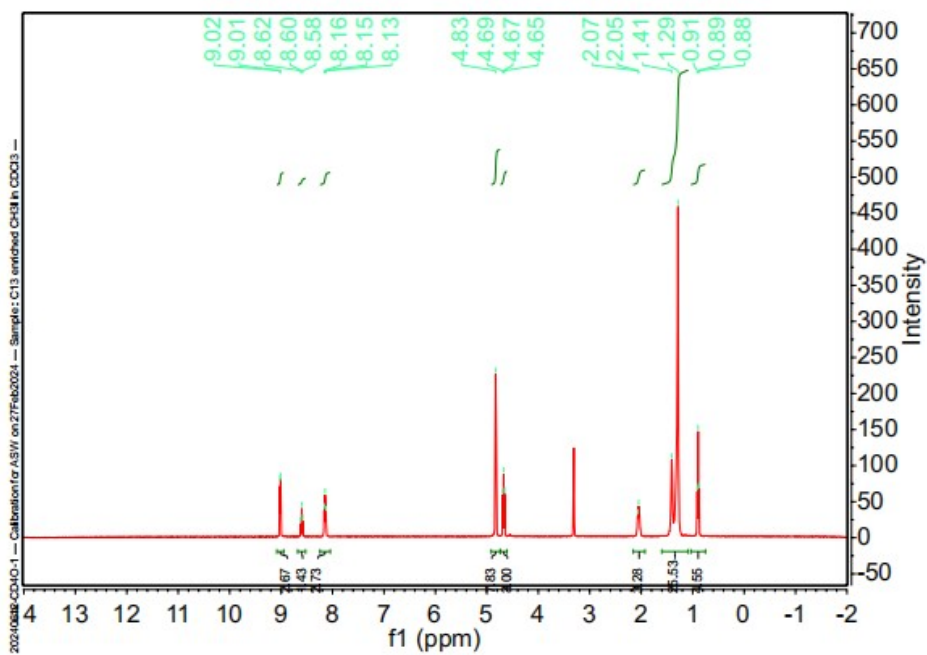


Figure S1.  $^1\text{H}$  NMR spectrum of  $[\text{C}_{12}\text{Py}]_3(\text{NH}_4)_3\text{Mo}_7\text{O}_{24}$  in  $\text{CD}_4\text{O}$ .

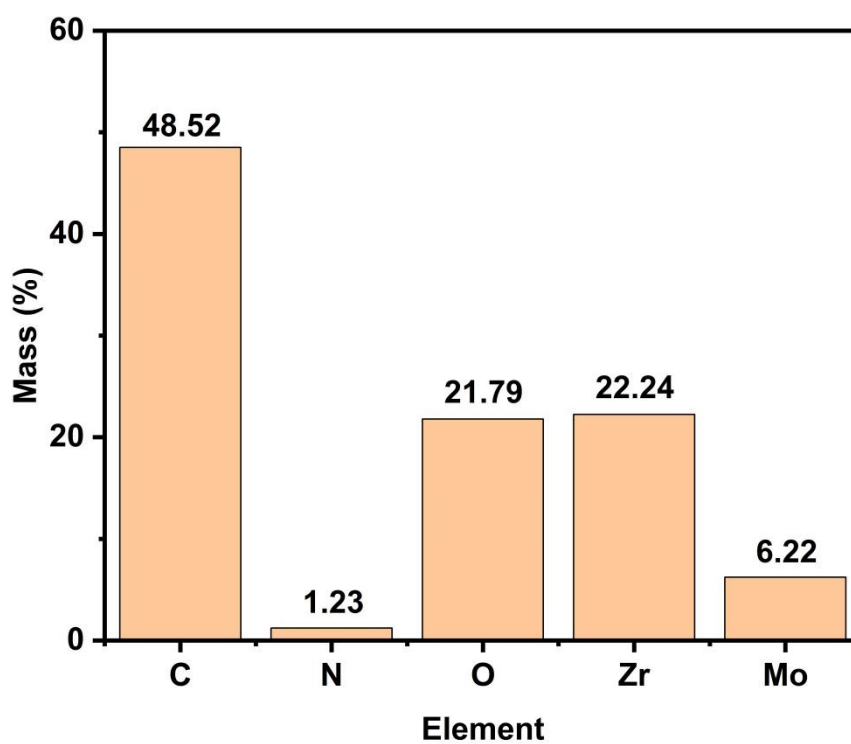


Figure S2. Quality percentage of different elements over  $C_{12}Py]_3(NH_4)_3Mo_7O_{24}/T-MOF-808-15\%$ .

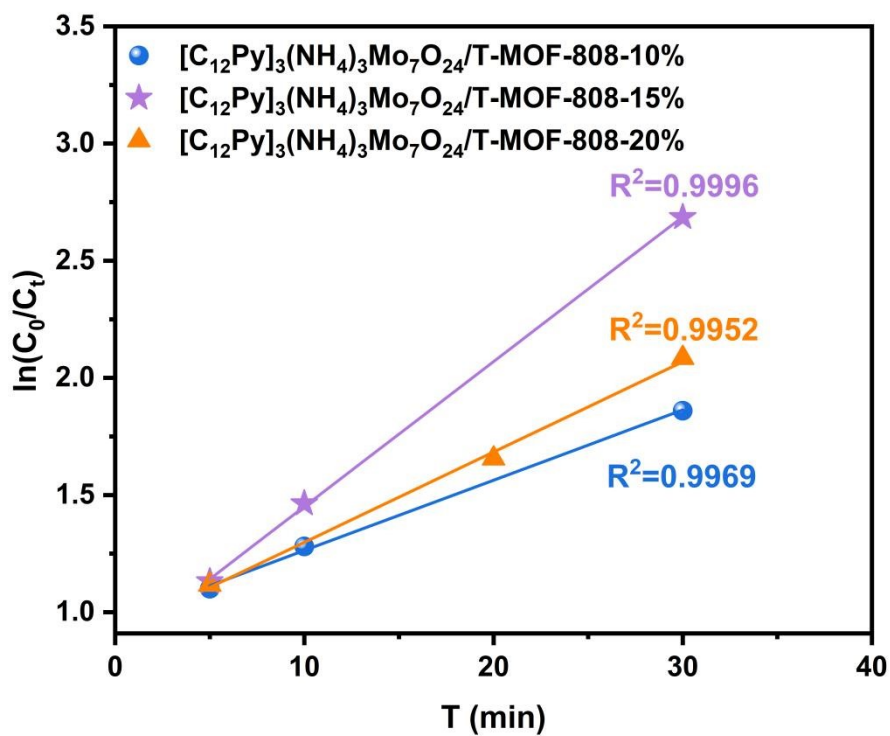


Figure S3. Pseudo-first-order kinetics for the oxidation of DBT at different loading amounts over  $[\text{C}_{12}\text{Py}]_3(\text{NH}_4)_3\text{Mo}_7\text{O}_{24}/\text{T-MOF-808}$ .

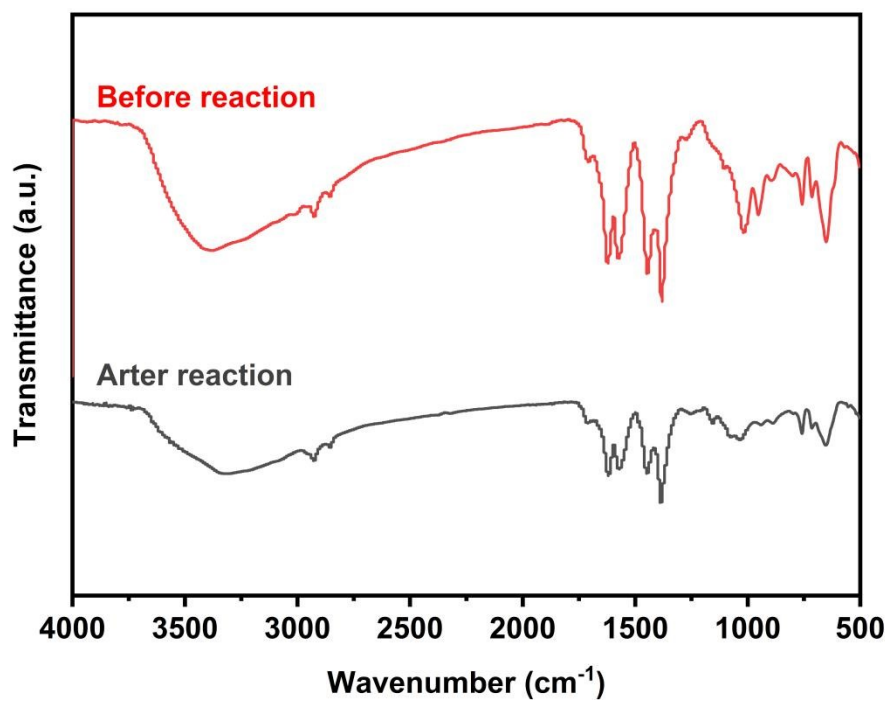


Figure S4. FT-IR spectra of  $[\text{C}_{12}\text{Py}]_3(\text{NH}_4)_3\text{Mo}_7\text{O}_{24}/\text{T-MOF-808-15\%}$  catalyst before and after reaction.

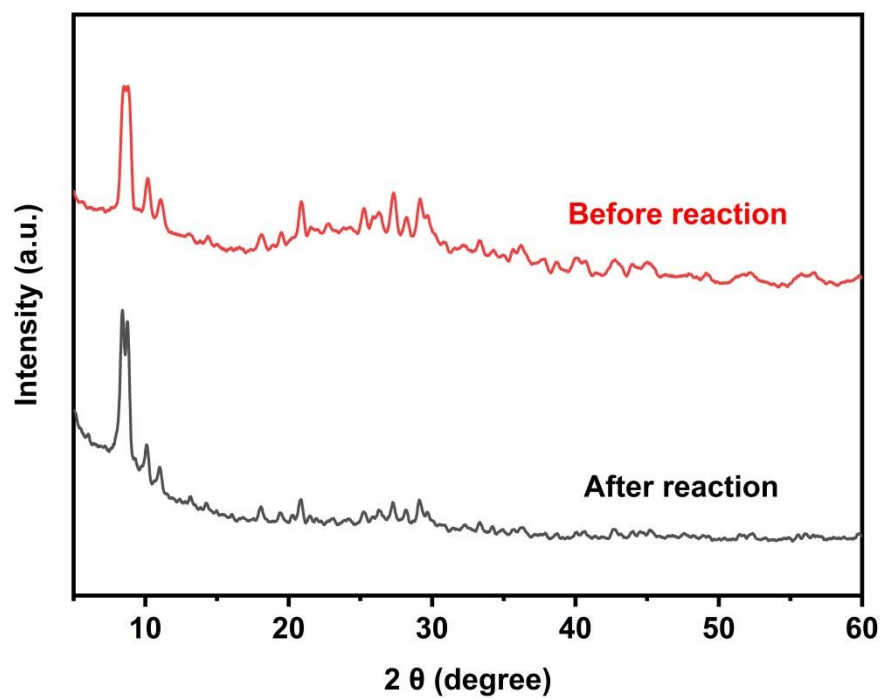


Figure S5. XRD patterns of  $[\text{C}_{12}\text{Py}]_3(\text{NH}_4)_3\text{Mo}_7\text{O}_{24}/\text{T-MOF-808-15\%}$  catalyst before and after reaction.

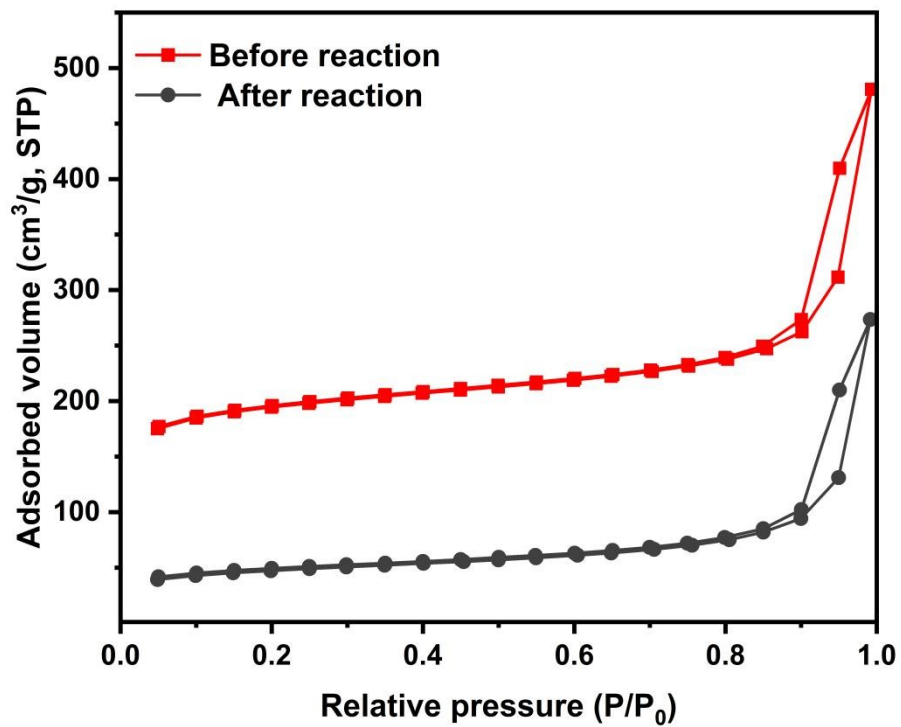


Figure S6.  $N_2$  adsorption-desorption isotherms of  $[C_{12}Py]_3(NH_4)_3Mo_7O_{24}/T-MOF-808$  before and after reaction.

**Table S1. Textural properties of different samples.**

Samples	BET surface area (m <sup>2</sup> /g)	Pore Volume (cm <sup>3</sup> /g)	Pore Diameter (nm)
MOF-808	924.78	0.81	3.05
T-MOF-808	899.89	0.74	3.06
[C <sub>12</sub> Py] <sub>3</sub> (NH <sub>4</sub> ) <sub>3</sub> Mo <sub>7</sub> O <sub>24</sub> /T-MOF-808-10%	687.21	0.65	17.45
[C <sub>12</sub> Py] <sub>3</sub> (NH <sub>4</sub> ) <sub>3</sub> Mo <sub>7</sub> O <sub>24</sub> /T-MOF-808-15%	497.83	0.63	30.99
[C <sub>12</sub> Py] <sub>3</sub> (NH <sub>4</sub> ) <sub>3</sub> Mo <sub>7</sub> O <sub>24</sub> /T-MOF-808-20%	205.77	0.31	17.35

**Table S2. Reaction rate constant corresponding to different loadings in the ODS reaction.**

Load capacity (%)	Rate constant <i>k</i> (min <sup>-1</sup> )	Correlation factor R <sup>2</sup>
10	0.02999	0.9969
15	0.06185	0.9996
20	0.03851	0.09952



**Table S3. Comparison of the ODS performances of different catalysts for DBT**

Entry	catalysts	Sulfur ( $\mu\text{g}\cdot\text{g}^{-1}$ )	Dosage (mg)	T ( $^{\circ}\text{C}$ )	O/S	t (min)	Conversi on rate (%)	Ref.
1	UIO-66	500	100	60	12	150	100	[1]
2	$\text{PMo}_{11}/\text{g-C}_3\text{N}_4$	100	100	30	10	20	98.6	[2]
3	UiO-66(Zr)-free	1000	50	60	6	120	99.6	[3]
4	$\text{Ti}_{32}$ -BTA	200	50	60	6	60	100	[4]
5	$\text{PW}_{12}@/\text{TiO}_2$	500	85	60	6	60	99.9	[5]
6	$[\text{C}_{12}\text{Py}]_3(\text{NH}_4)_3\text{Mo}_7\text{O}_{24}/\text{T-MOF-808-15\%}$	500	100	60	6	40	100	This work

## References

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