

Electronic Supplementary Information

Shape-controlled synthesis of metal-organic framework MIL-125 towards highly enhanced catalytic performance for oxidative desulfurization of 4,6-dimethyldibenzothiophene

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Table 1. Textural properties of the MIL-125 and MIL-125-TRO.

| Sample | S_{BET} (m^2/g) ^a | S_{ext} (m^2/g) ^b | V_{total} (cm^3/g) | V_{micro} (cm^3/g) ^b | $V_{\text{micro}}/ V_{\text{total}}$ |
|-------------|---------------------------------------------------------|---------------------------------------------------------|-----------------------------------------------|------------------------------------------------------------|--------------------------------------|
| MIL-125 | 1181 | 165 | 0.61 | 0.50 | 0.82 |
| MIL-125-TRO | 1320 | 181 | 0.67 | 0.55 | 0.82 |

^aSpecific surface area calculated using the BET method.

^b S_{ext} (external surface area) and V_{micro} (micropore volume) calculated using the *t*-plot method.

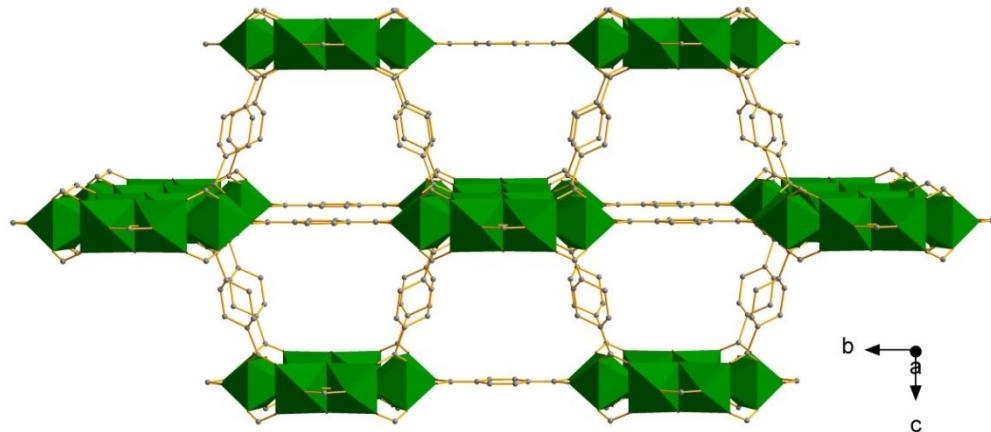


Fig. S1 Representation of the structure of MIL-125.

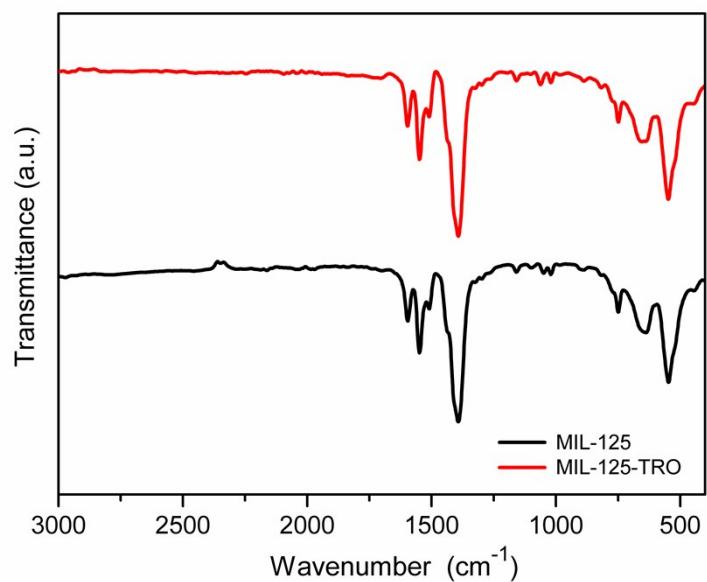


Fig. S2 IR spectra of MIL-125 and MIL-125-TRO.

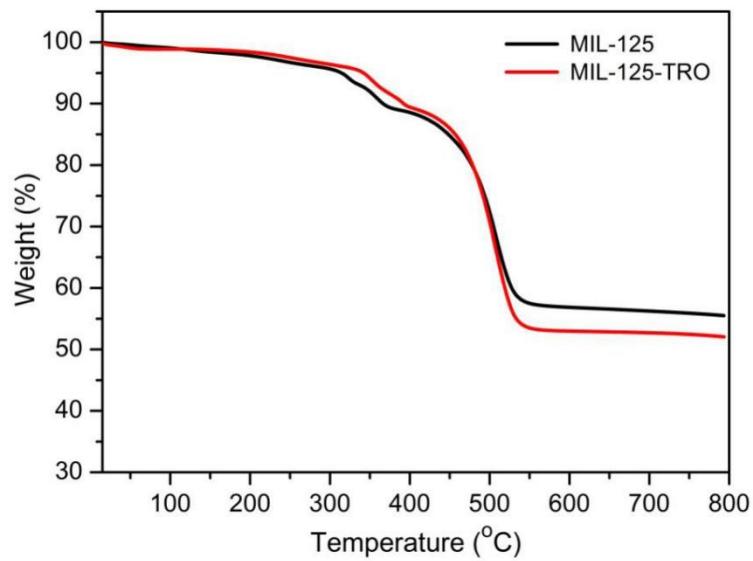


Fig. S3 TGA curves of MIL-125 and MIL-125-TRO.

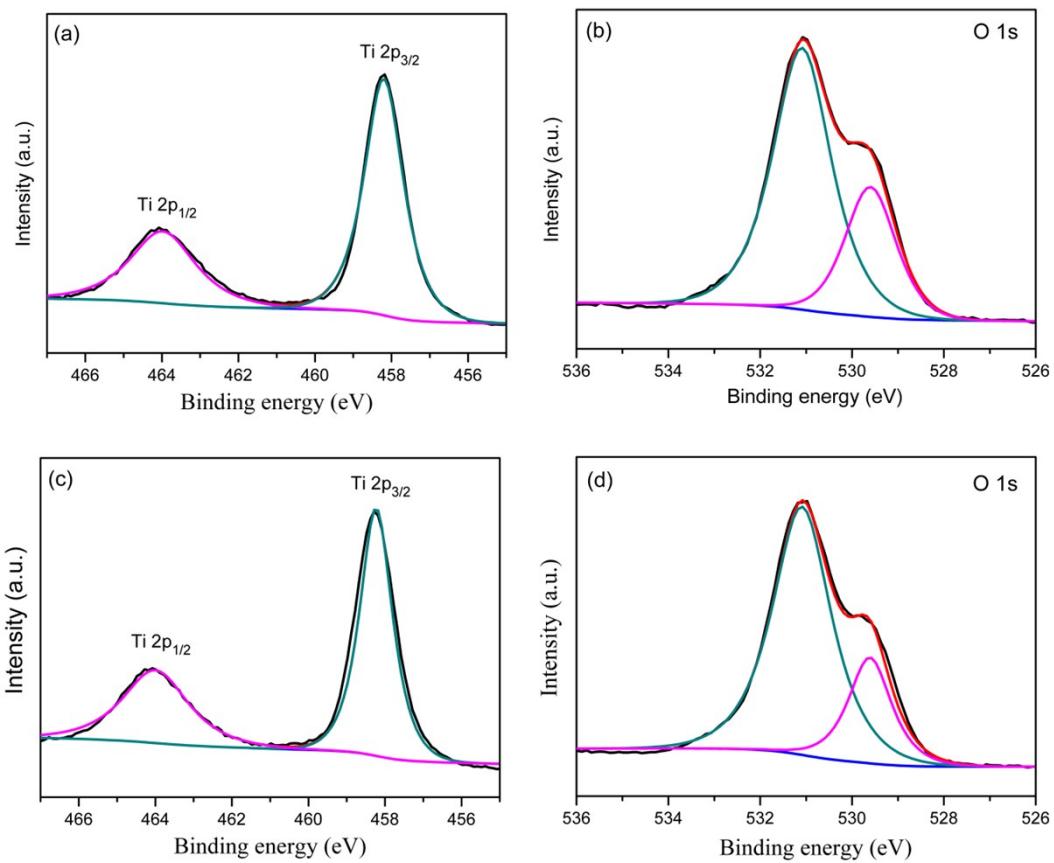
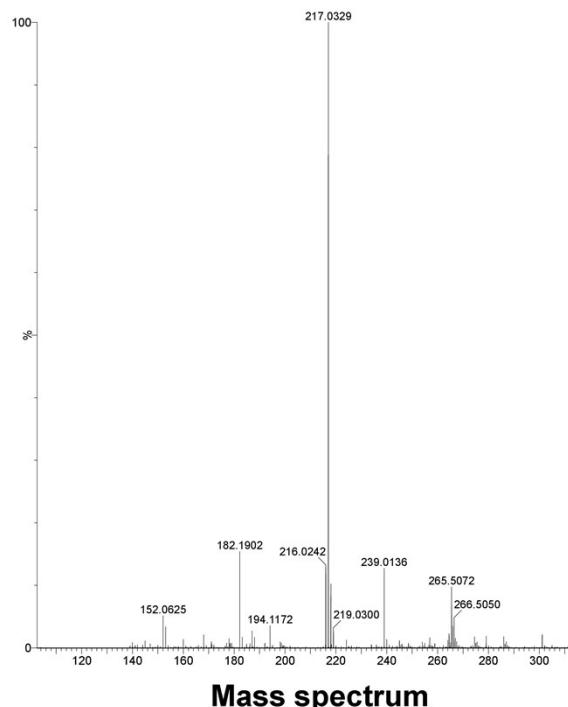
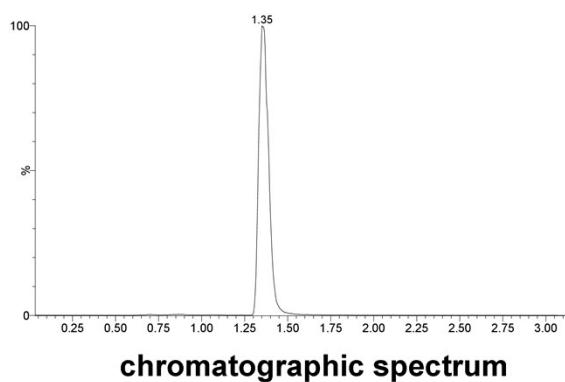


Fig. S4 Ti 2p XPS spectra of (a) MIL-125 and (c) MIL-125-TRO; O 1s XPS spectra of (b) MIL-125 and (d) MIL-125-TRO.

(a)



(b)

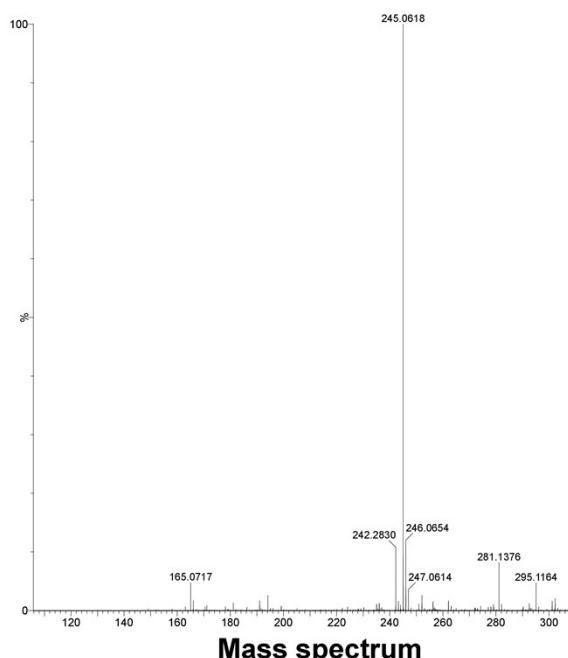
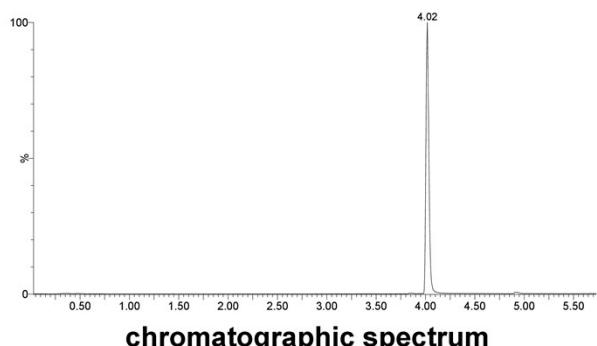


Fig. S5 LC-MS analysis of the products for ODS of (a) DBT and (b) 4,6-DMDBT.

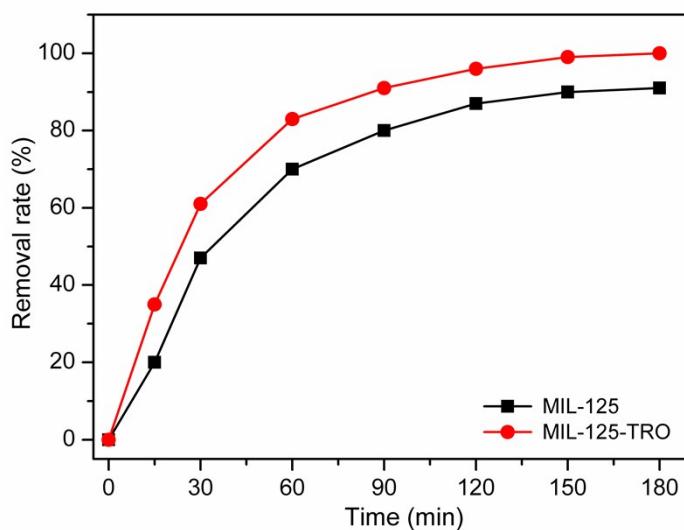


Fig. S6 Oxidative desulfurization of Th over MIL-125 and MIL-125-TRO catalysts.

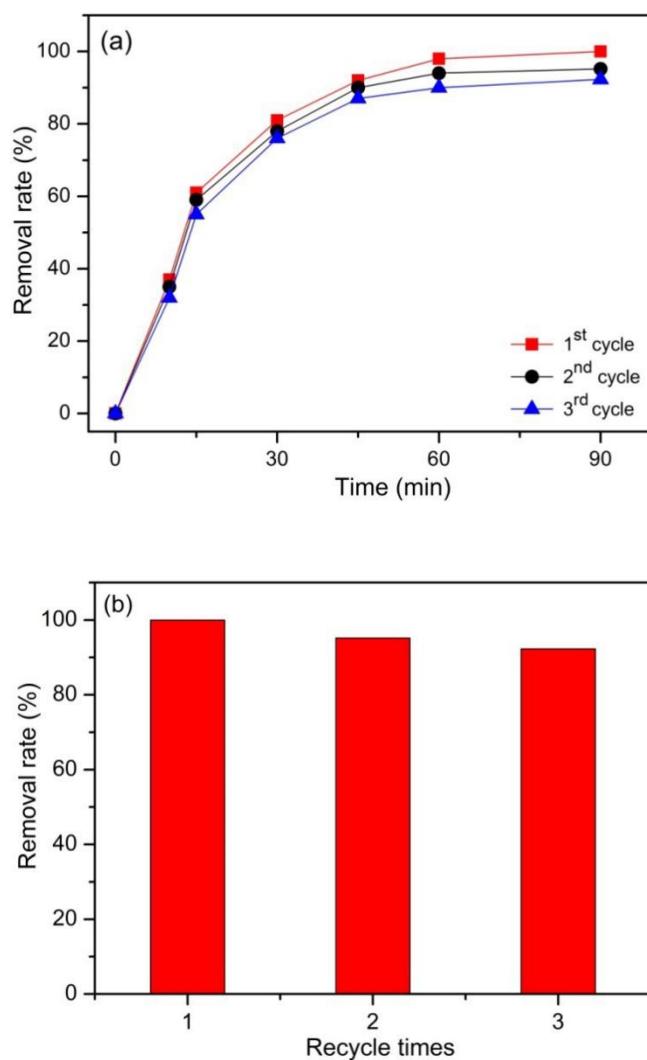


Fig. S7 (a) Kinetic profiles and (b) final removal rates for three consecutive ODS cycles of 4,6-DMDBT over MIL-125-TRO catalyst.

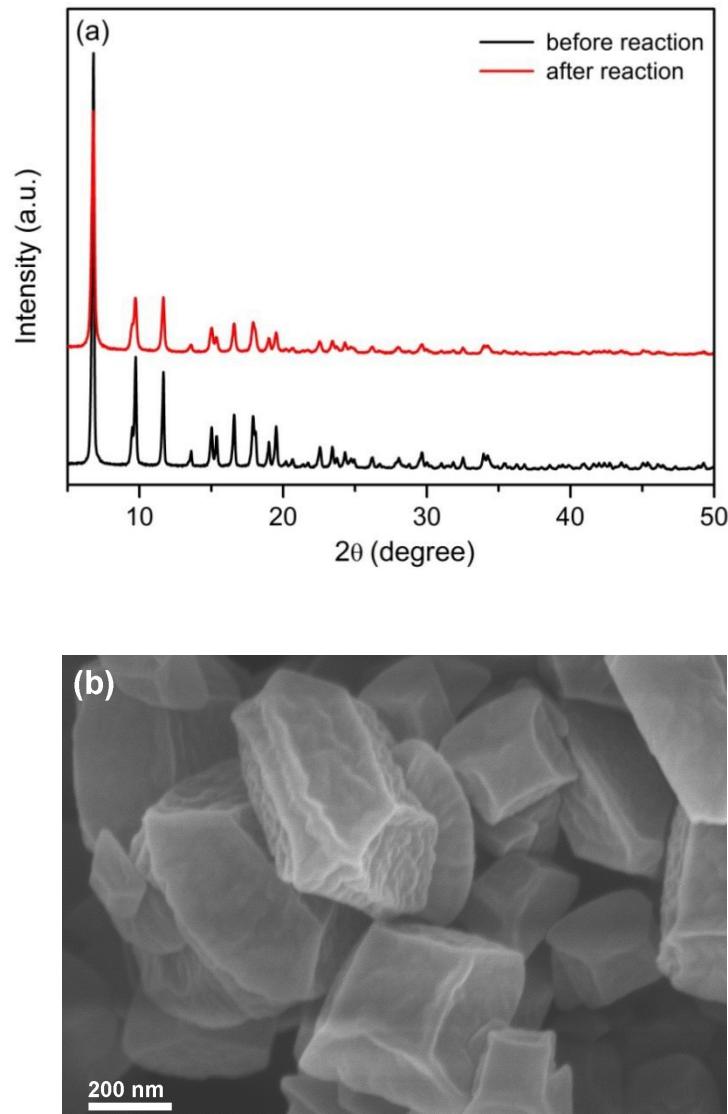


Fig. S8 (a) PXRD patterns and (b) SEM image of MIL-125-TRO after three consecutive cycles for ODS of 4,6-DMDBT.