Supplementary materials

A Nut-like MOF/Hydroxylated Graphene Hybrid Materials for Adsorptive Desulfurization of Thiophene

Ke YANG,*† Yu YAN,† Wen CHEN,† Hongtao KANG,† Yi HAN,† Wenquan ZHANG,† Yafeng Fan* and Zhenxing LI*†

a State Key Laboratory of Heavy Oil Processing, Institute of New Energy, China University of Petroleum-Beijing, Beijing, 102249, P. R. China.
† These authors contributed equally.

Fig. S1 The SEM, EDS O-Ka (red) and C-Ka (yellow) images of HG.

Fig. S2 EDS line scanning and element content of Cu (blue), O (green) and C (red) for MGr-5 composite.
**Fig. S3** The possible interactions between Cu-BTC and hydroxyl groups of HG: (a) the HG dispersed on the surface of Cu-BTC crystal, and (b) the HG inserted inside Cu-BTC crystal to lead to the alternated growth of Cu-BTC and graphene layers.

**Table 1**

| Element | Wt%  | At%  |
|---------|------|------|
| CK      | 30.37| 55.06|
| OK      | 21.67| 28.73|
| CuK     | 47.96| 16.20|
| **Matrix** | **Correction** | **ZAF** |

**Fig. S4** The EDS analyses for Cu-BTC and MGr-5 composite with elemental content of C, O and Cu in surface of material, respectively.
Fig. S5. The FT-IR spectrum of HG.

Fig. S6. The Langmuir plots for T adsorption by HG

Calculation of maximum sulfur adsorption capacity ($Q_0$):

The maximum sulfur adsorption capacity of all samples were calculated according to the Langumir adsorption isotherm. The linear form of Langmuir's isotherm mode was plotted by the following equation[1]:

$$\frac{C_e}{q} = \frac{C_e}{Q_0} + \frac{1}{Q_0 b}$$

Where,

$C_e$: equilibrium sulfur concentration in model oils (ppm)

$q$: adsorption capacity of adsorbent (mg-S/g)
Q₀: Langmuir constant (maximum sulfur adsorption capacity, mg-S/g)

b: Langmuir constant (L/mg)

Thus, the maximum sulfur adsorption capacity can be gained by the reciprocal of the slope of the plot of $C_e/q$ against $C_e$.

![Fig. S7. The X-ray diffraction patterns of Cu-BTC and MGr-3 composite after fifth regeneration.](image)

1. B.H. Hameed, D.K. Mahmoud, A.L. Ahmad, *Journal of hazardous materials*, 2008, **158** 65-72.