

Supplementary Information

Ultradeep hydrodesulfurization of fuel over superior NiMoS phases
constructed by novel $\text{Ni}(\text{MoS}_4)_2(\text{C}_{13}\text{H}_{30}\text{N})_2$ precursor

Jundong Xu, Chenglong Wen, Shuisen He, Yu Fan*

State Key Laboratory of Heavy Oil Processing, China University of Petroleum,
Beijing 102249, P.R. China

* Corresponding author. Tel.: +86 10 89734981; fax: +86 10 89734979.

E-mail address: fanyu@cup.edu.cn (Y. Fan)

Table S1 Properties of FCC diesel.

Item	Value
Density (20 °C) (g·cm ⁻³)	0.856
Sulfur (μg·g ⁻¹)	3640
Kinematic viscosity (20 °C) (mm ² ·s ⁻¹)	5.39
Cetane number	39
Distillation (ASTM D86) (°C)	
IBP	210
10%	249
50%	296
90%	342
FBP	363

The typical HRTEM images of s-NiMo/ γ -Al₂O₃-DE and s-NiMo/ γ -Al₂O₃-D are shown in Fig. S1. Most of MoS₂ slabs on s-NiMo/ γ -Al₂O₃-DE (Fig. S1a) have the same length and stacking layer number as those of s-NiMo/ γ -Al₂O₃-D (Fig. S1b). In addition, s-NiMo/ γ -Al₂O₃-DE has almost the same distributions of lengths (Fig. S1c) and stacking layer numbers (Fig. S1d) of the MoS₂ slabs as those of s-NiMo/ γ -Al₂O₃-D.

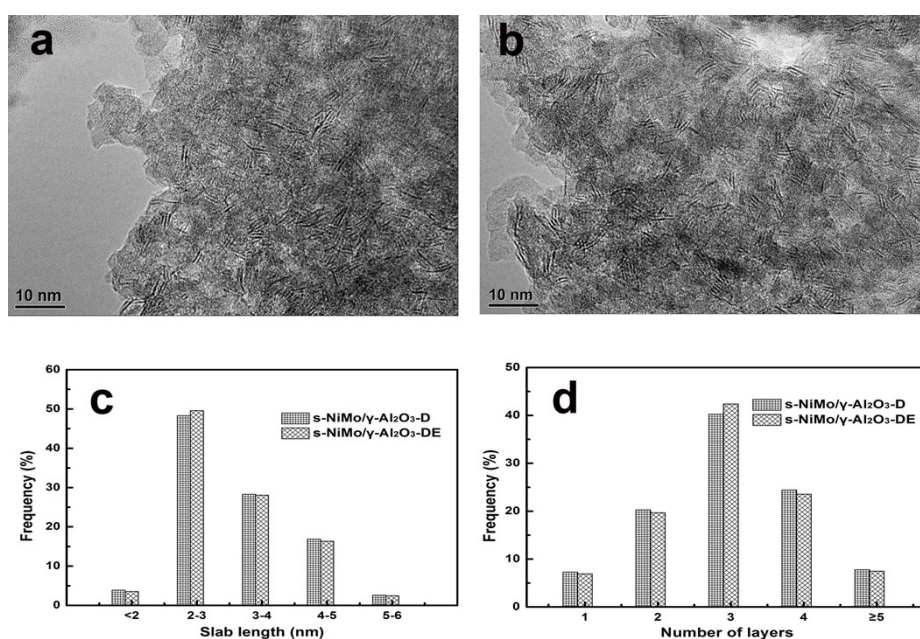


Fig. S1. HRTEM images of s-NiMo/ γ -Al₂O₃-DE (a), s-NiMo/ γ -Al₂O₃-D (b); statistical distributions of the lengths (c) and stacking numbers (d) of MoS₂ slabs on s-NiMo/ γ -Al₂O₃-DE and s-NiMo/ γ -Al₂O₃-D.

The reaction rate constants (k_{HDS}) and TOF values of s-NiMo/ γ -Al₂O₃-D (prepared using alumina powder as a support) and s-NiMo/ γ -Al₂O₃-DE (prepared using alumina extrude as a support) for 4,6-DMDBT HDS are listed in Table S2. s-NiMo/ γ -Al₂O₃-DE has almost the same k_{HDS} (6.32×10^{-7} mol g⁻¹ s⁻¹) and TOF value (9.98×10^{-4} s⁻¹) as those of s-NiMo/ γ -Al₂O₃-D.

Table S2 HDS results for 4,6-DMDBT on s-NiMo/ γ -Al₂O₃-D and s-NiMo/ γ -Al₂O₃-DE.

Catalyst	k_{HDS} (10^{-7} molg ⁻¹ s ⁻¹)	TOF $\times 10^4$ (s ⁻¹)
s-NiMo/ γ -Al ₂ O ₃ -D	6.35	10.01
s-NiMo/ γ -Al ₂ O ₃ -DE	6.32	9.98