

## **Supporting Information for**

# **SDBS-assisted hydrothermal synthesis of flower-like Ni-Mo-S catalysts and their enhanced hydrodeoxygenation activity**

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### **Experimental Details**

#### **Preparation of catalysts**

All solvents and reagents were obtained from Sinopharm Chemical Reagent Co., Ltd. in high purity ( $\geq 99\%$ ) and used without further purification. The catalyst synthesis was carried out in quartz reactor with a volume of 300 mL. Ammonium heptamolybdate (2.32 g), nickel nitrate (1.14 g), SDBS (0, 0.1, 0.2, 0.3 g, 0.4 g) and thiourea (3.00 g) were dissolved in 250 mL water and hydrochloric acid was added to adjust its pH value to 0.8. Then, this mixed solution was added into the sealed reactor and heated at 200 °C for 12 hours. After reaction, the resultant catalysts were separated and washed with water and ethanol for several times. Finally, the resulting product was dried under vacuum at 60 °C for 5 hours and denoted as Ni-Mo-S-X, where X represented the added weight (g) of SDBS.

#### **Catalyst characterization**

The specific surface area was measured by a Quantachrome's NOVA-2100e Surface Area instrument by physisorption of nitrogen at -196 °C. The samples were dehydrated at 300 °C using vacuum degassing for 12 h before experiments. X-ray diffraction (XRD) measurements were carried on a D/max2550 18KW Rotating anode X-Ray Diffractometer with monochromatic Cu K $\alpha$  radiation ( $\lambda = 1.5418 \text{ \AA}$ ) radiation at voltage and current of 40 kV and 300 mA. The  $2\theta$  was scanned over the range of 10-90° at a rate of 10°/min. The scanning electronic microscopy (SEM) images of the catalysts were obtained on a JEOL JSM-6360 electron microscopy. The morphology was determined by high resolution transmission electron microscopy (HRTEM) on a JEOL JEM-2100 transmission electron microscope with a lattice resolution of 0.19 nm and an accelerating voltage of 200 kV. The samples

for the HRTEM study were prepared by the ultrasonic dispersing in ethanol and consequent deposition of the suspension upon a “holey” carbon film supported on a copper grid. The samples were kept under inert atmosphere until the last process.

### **Catalyst activity measurement**

The HDO activity tests were carried out in a 100-mL sealed autoclave. The prepared catalyst (0.2 g) without any further treatment, *p*-cresol (6.4 g) and dodecane (26 g) were placed into the autoclave. Air in the autoclave was evacuated by pressurization-depressurization cycles with nitrogen and subsequently with hydrogen. The system was heated to 275 °C, then pressurized with hydrogen to 4.0 MPa and adjusted the stirring speed to 900 rpm. During the reaction, liquid samples were withdrawn from the reactor and analysed by Agilent 6890/5973N GC-MS and 7890 gas chromatography using a flame ionization detector (FID) with a 30 m AT-5 capillary column. The experiments have been repeated twice at least and the results showed that the conversion and selectivity were within 3.0% of the average values. The deoxygenation degree and HYD/DDO for each experiment were calculated as follows:

$$\begin{aligned} & \text{Deoxygenation degree (D. D., wt\%)} \\ & = \left(1 - \frac{\text{oxygen content in the final organic compounds}}{\text{total oxygen content in the initial material}}\right) \times 100 \% \end{aligned}$$