Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Ni-promoted MoS_2 in Hollow Zeolite Nanoreactors: Enhanced Catalytic activity and stability for Deep Hydrodesulfurization

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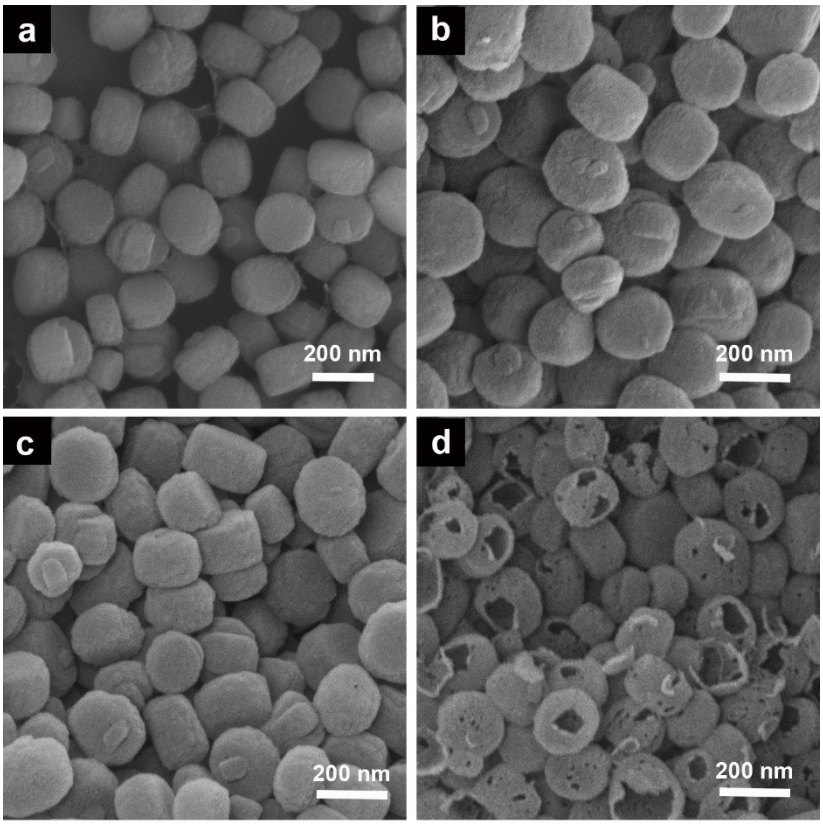

Figure S1. SEM images of ZSM-5 after 0.2 M NaOH aqueous solution treatment for different times: 0 min (a), 15 min (b), 45 min (c) and 60 min (d).

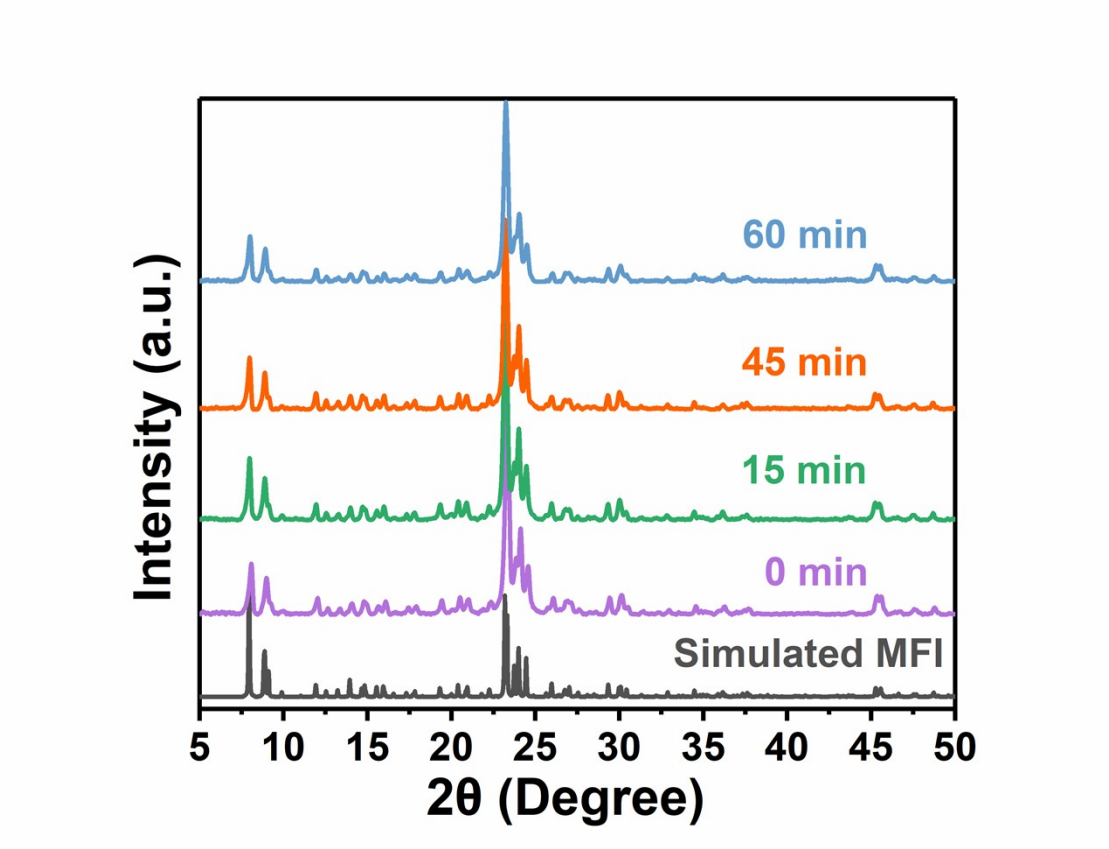

Figure S2. Wide-angle XRD of ZSM-5 zeolite with different alkaline solution treatment time (0 min, 15min, 45min and 60min).

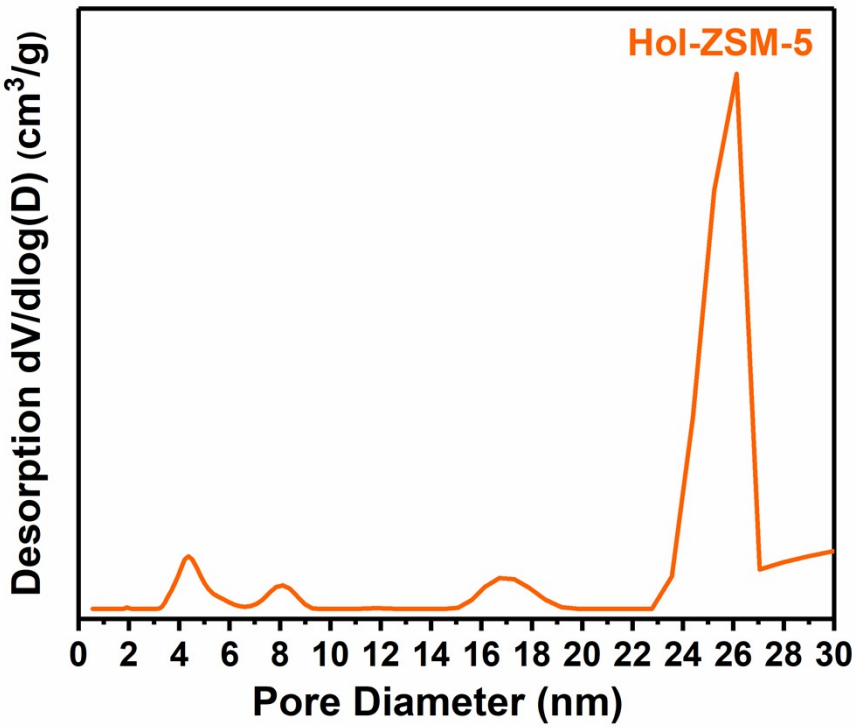

Figure S3. Pore size distribution of Hol-ZSM-5 zeolite

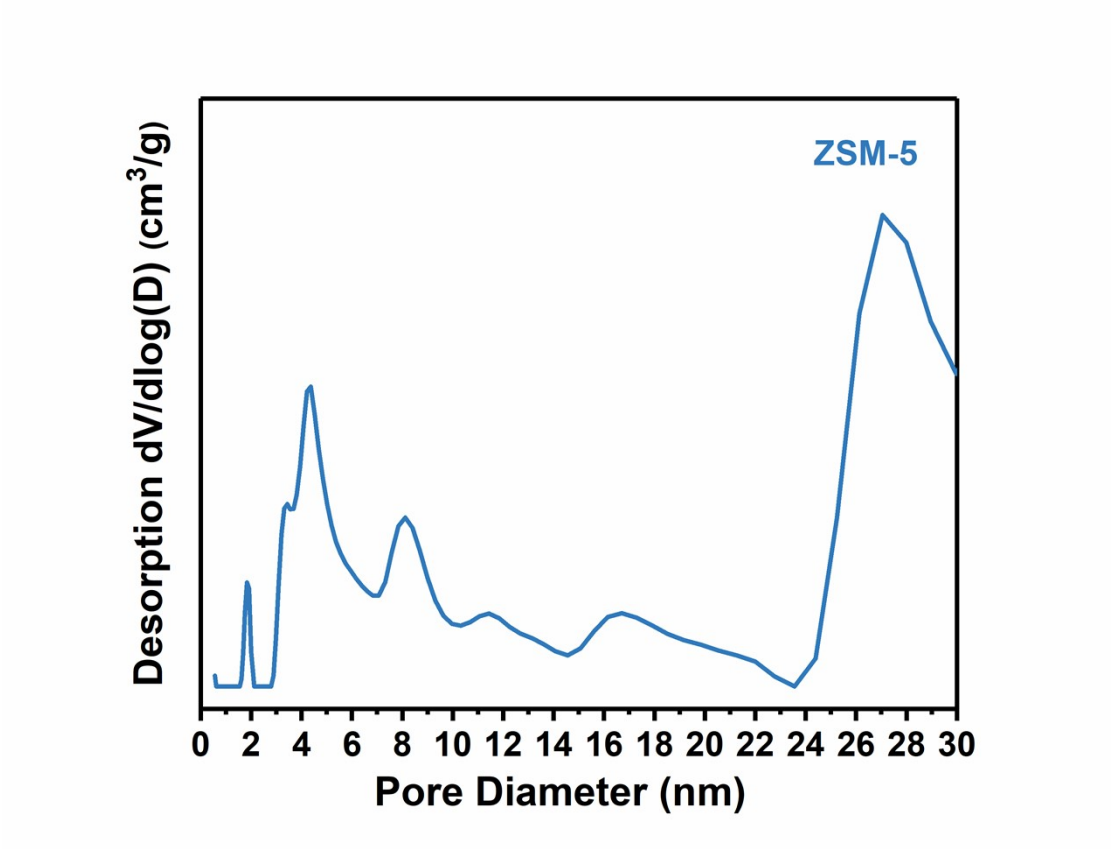

Figure S4. Pore size distribution of ZSM-5 zeolite

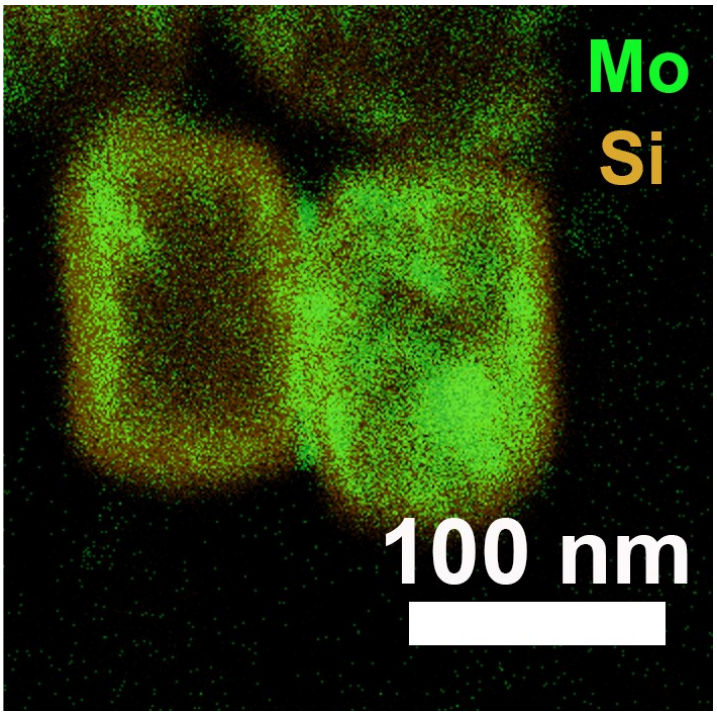

Figure S5. The EDS mapping for Si and Mo elements in $NiMoS_X$/Hol-ZSM-5 catalyst.

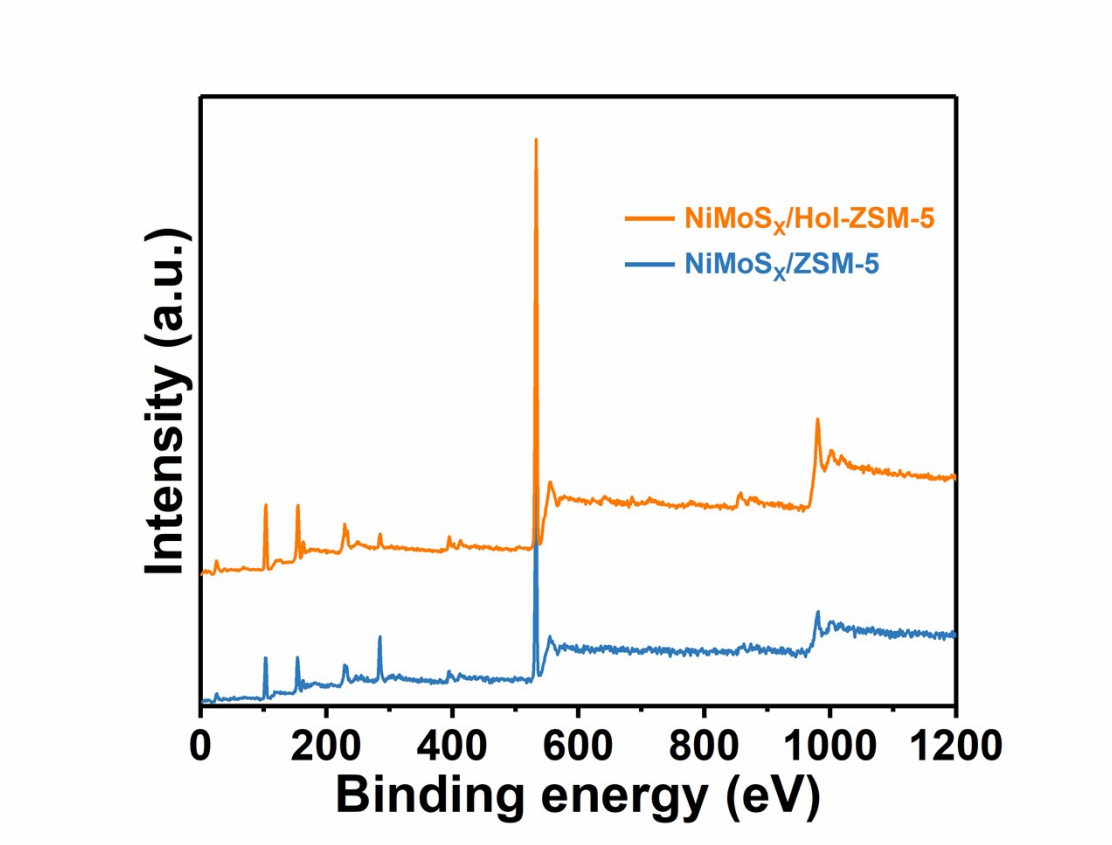

Figure S6. XPS survey spectra of the $NiMoS_X$/Hol-ZSM-5 and $NiMoS_X$/ZSM-5 catalysts.

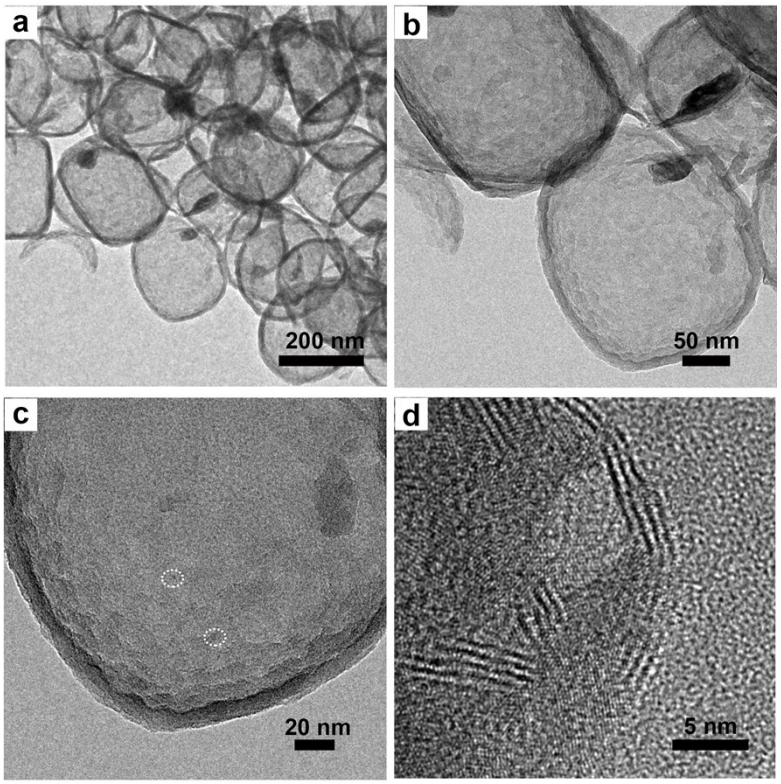

Figure S7. TEM images of $NiMoS_X$/Hol-ZSM-5 catalyst after HDS catalysis testing for 80 h.

Table S1. Textural parameters of Hol-ZSM-5 and ZSM-5 supports.

Sample	S_{BET} (m^2g^{-1})[a]	V_{Total} (cm^3g^{-1})[b]	V_{Micro} (cm^3g^{-1})[c]	Average pore width (nm)[d]
ZSM-5	536.6	0.614	0.098	0.56
Hol-ZSM-5	332.4	1.327	0.033	27.4

[a] BET Surface area
[b] Total pore volume, $P/P_0 = 0.989$
[c] t-Plot method
[d] DFT pore diameter

Table S2. Ni 2p XPS spectra of $NiMoS_X$/Hol-ZSM-5 and $NiMoS_X$/ZSM-5 catalysts.

Catalysts	NiS_X		$NiMoS_X$		NiO	
	BE (eV)	ar.%	BE (eV)	ar.%	BE (eV)	ar.%
$NiMoS_X$/Hol-ZSM-5	852.5±0.1	10.03	855.9±0.1	82.06	860.1±0.1	7.91
$NiMoS_X$/ZSM-5	852.5±0.1	10.62	855.9±0.1	73.36	860.1±0.1	16.02

Table S3. Mo 3d XPS spectra of $NiMoS_X$/Hol-ZSM-5 and $NiMoS_X$/ZSM-5 catalysts.

Catalysts	Mo^{4+}		Mo^{5+}		Mo^{6+}		S_{Mo} [b]
BE (eV)	ar.%	ar.%	ar.%	ar.%	ar.%	ar.%	
	229.3 ±0.1	232.3 ±0.1	231.2 ±0.1	234.6 ±0.1	233.3 ±0.1	236.3 ±0.1	
$NiMoS_X$/Hol-ZSM-5	51.69	33.53	1.26	0.84	7.59	5.09	85.22%
$NiMoS_X$/ZSM-5	45.07	27.32	14.26	10.31	2.28	0.76	72.39%

[a] ar.% indicates the area percent of XPS peak. [b] $S_{Mo} = Mo_{sulfidation} = Mo^{4+}/(Mo^{4+}+Mo^{5+}+Mo^{6+})$

Table S4. DBT HDS performance of $NiMoS_X$/Hol-ZSM-5 and $NiMoS_X$/ZSM-5 catalysts.

Catalysts	Conversion[a] (%)	k_{HDS} (mol·g^{-1}·s^{-1})	Product selectivity[b] (%)			DDS/HYD ratio
			HYD	DDS		
			DCH	CHB	BP	
$NiMoS_X$/Hol-ZSM-5	30.26	18.74×10^{-7}	0.19	2.57	97.24	35.23
$NiMoS_X$/ZSM-5	29.89	5.54×10^{-7}	2.25	17.46	80.29	4.74

[a]The DBT HDS conversion was obtained by changing the WHSV (330 °C, 4 MPa, hydrogen-oil ratio of 600).
[b]Definition at a total DBT conversion of 30% by changing the WHSV.