Synergistic effect of acidity and active phases on DBT HDS performance: the role of S-edge and Mo-edge sites

Zhengkai Cao[1], Xia Zhang[2], Rong Guo[2], Chong Peng[3], Peng Zheng[1], Xilong Wang[4], Jiyuan Fan[1], Jinlin Mei[1], Chunming Xu[5], and aijun duan[6]

[1]China University of Petroleum Beijing
[2]Fushun Research Institute of Petroleum and Petrochemicals
[3]East China University of Science and Technology
[4]China University of Petroleum Beijing College of Chemical Engineering
[5]Chinese University of Petroleum
[6]China University of Petroleum, Beijing

May 5, 2020

Abstract

Dual-metal modifications on SBA-16 silica were implemented to modulate the acidities and the distribution and dispersion of active phases for NiMo catalysts. The results showed that the acidity of S-H groups in S-edge sites can be promoted by B acid and further facilitate the DDS selectivity. The NiMo/AT-7.5 catalyst exhibits the highest HDS efficiency of 97.5% due to its appropriate acidity, highest proportion of MoS2 phase and concentration of S-edge sites. The kinetic and thermodynamic analyses were applied to investigate the intrinsic HDS reactivity for various catalysts. The results confirmed the existence of synergistic effect in the DBT HDS reaction. The B acid sites can further increase the desulfurization route (DS) of THDBT to CHB. A higher dispersion degree of MoS2 could improve DBT HDS efficiency. A high total concentration of S-edge and Mo-edge will indicate a high HDS efficiency. The S-edge/Mo-edge ratio and kDDS/kHYD could be correlated.

Hosted file

`zhengkai cao submitted manuscript to AICHE - revised.pdf` available at https://authorea.com/users/295949/articles/424809-synergistic-effect-of-acidity-and-active-phases-on-dbt-hds-performance-the-role-of-s-edge-and-mo-edge-sites