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One Pot Synthesis of Ultrasmall NiMo Catalysts Supported on Amorphous Alumina with Enhanced type 2 Sites for Hydrodesulfurization Reaction: A Combined Experimental and Theoretical Study

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Abstract : The deep removal of high molecular weight sulphur compounds (e.g., 4,6, dimethyl dibenzothiophene) is challenging due to their steric hindrance. Hydrogenation desulfurization (HYD) pathway is the main pathway to remove these sulfur compounds, and it is mainly governed by the number of type 2 sites. The formation of type 2 sites can be enhanced by modulating the pore structure and the interaction between the active metal and support. To this end, we report the enhanced HDS catalytic activity of ultrasmall NiMo supported on amorphous alumina (A-Al_2O_3) catalysts by one pot colloidal synthesis method followed by calcination and sulfidation. The amorphous alumina (A-Al_2O_3) was chosen as the support due to its lower surface energy, better physicochemical properties, and enhanced acidic sites (due to the dominance of tetra and penta coordinated [Al] sites) than crystalline alumina phase. At 20% metal oxide composition, NiMo supported on A-Al_2O_3 catalyst showed 1.4 and 1.2 times more reaction rate constant and turn over frequency (TOF) respectively than the conventional catalyst (wet impregnated NiMo catalysts) for HDS reaction of dibenzothiophene reactant molecule. A-Al_2O_3 supported catalysts represented enhanced type 2 sites formation (because this catalystpossesses higher sulfidation degree (80%) and NiMoS sites (19.3 x 10^{17} sites/mg) with desired optimum stacking degree (2.5) than wet impregnated catalyst at same metal oxide composition 20%) along with higher active metal dispersion, Mo edge site fraction. The experimental observations were also supported by DFT simulations. Lower heat of adsorption (< 4.2 ev for MoS2 interaction and < 3.15 ev for Ni doped MoS2 interaction) values for A-Al_2O_3 confirmed the presence of weaker metal-support interaction in A-Al_2O_3 in contrast to crystalline ɣ-Al_2O3. The weak metal-support interaction for prepared catalysts clearly suggests the higher formation of type 2 sites which leads to higher catalytic activity for HDS reaction.

Keywords : amorphous alumina, colloidal, desulfurization, metal-support interaction
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