Experimental and computational studies of sulfided NiMo supported on pillared clay: catalyst activation and guaiacol adsorption sites

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Abstract	We report on intermediate (oxysulfides) and sulfided structures of NiMo supported on aluminium pillared clay (Al-PILC) during the catalyst activation process and the prefered guaiacol adsorption sites on the sulfided catalyst. In situ X-ray absorption fine structure (XAFS) together with density functional theory (DFT) calculations confirm the existence of ill-defined suboxides (MoOx, NiOx) and the well-known subsulfides (Mo2S9, Ni3S2) at the first stage which, at a later stage in the process, transform into MoS2 with two edges, oxygen-decorated Mo and Ni with zero sulfur coverage. The freshly sulfided NiMoS2 catalyst under sulfiding agents is mainly terminated by Mo-edge surface with 50% sulfur coverage (Mo-S50) with a disordered Ni-edge surface that can be assigned as NiMoS (1010). When exposed to an inert atmosphere such as He gas, the Mo and Ni edges evolved partially into new structures of Mo and Ni edges with zero sulfur coverage, labelled as Mo-Bare and Ni-Bare. Guaiacol is often used as a model compound for lignin and a series of calculations of guaiacol on the structural edges of a sulfided NiMoS2 catalyst show relatively good agreement between the observed and calculated inelastic neutron scattering (INS) spectra for Mo-S50, Ni-Bare, and NiMoS (1010) where guaiacol weakly chemisorbed via oxygen atom of OH group. The results also confirm that guaiacol is physisorbed on the basal plane of NiMoS2 in a horizontal (flat-lying) configuration via van der Waals interaction at a separation of about 3.25 angstrom.
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