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A DFT comparative study of the stability of zeolite-supported molybdenum and niobium sulfide catalysts promoted by Co and Ni along the thiophene hydrodesulfurization reaction pathway

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The relative stabilities, along the thiophene hydrodesulfurization reaction pathways, of the intermediate nanostructures of molybdenum and niobium sulfide catalysts promoted by Co and Ni and supported on zeolites (mordenite, 3-D structure) are compared by means of DFT calculations. The calculations explore the stability of the extra-framework promoted nanostructures anchored on an acidic site of the mordenite for the different steps of the reaction with H₂ and H₂S. In particular these stabilities are examined for the intermediate structures in the HYD (3, 4) and (2, 5) pathways and also along the DDS pathway. For the latter, it is observed that the niobium sulfide catalyst promoted by Co shows a greater stability than the Co-promoted MoS₂ catalyst. A similar situation is also observed for the case when Ni is the promoter. Similar results are obtained for the other reaction pathways.