Dynamic ab initio study towards new hydrocarbon pool cycles for the MTO-conversion in H-SAPO-5.

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Waning oil reserves emphasize the necessity of innovation to continue the supply of base chemicals like ethylene and propylene. The methanol-to-olefins process (MTO) is a promising alternative for olefin production, as syngas can be produced from different sources other than oil and can subsequently be converted to methanol.[1]

Overall, it is accepted that the reaction occurs through a hydrocarbon pool (HP) mechanism. Hydrocarbons, occluded in the pores of the zeolite or zeotype catalyst, act as co-catalysts during methanol conversion. The structure of the most reactive HP component depends on both the topology and the chemical composition of the catalyst.[2],[3]

In this contribution, we study the MTO process in H-SAPO-5 and H-SSZ-24, exhibiting the AFI topology. The large 1D channels which are present are open to a wide range of hydrocarbon feeds. This allows detailed mechanistic studies as a variety of HP species can be co-fed together with methanol. Molecular simulations are a potent tool to evaluate and comprehend the complex experimental results.[2],[3]

The influence of the methanol loading and framework composition on the adsorption of methanol and benzene in H-SAPO-5 and H-SSZ-24 are evaluated using periodic DFT based simulations. Various possibilities for adsorption complexes are investigated. The isostructural materials induce important differences in the preferential guest molecule-framework interaction due to their different chemical composition.

Additionally, crucial reaction steps like olefin elimination and methylation reactions are studied by means of a molecular dynamics approach, which provides insight in the reactivity of the different adsorption complexes and allows to investigate temperature effects.[4]

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