

## **Ab initio study on the deactivation of zeolite and zeotype catalysts during the MTO process**

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The depletion of oil reserves and the rapidly increasing demand for ethylene and propylene initiated the quest for chemical processes based on alternative feedstock. Among these, the methanol-to-olefin process (MTO), using natural gas, coal or biomass as raw material, is one of the most important. MTO conversion occurs in acidic zeolites or zeotype catalysts.

The generally accepted reaction mechanism for MTO is based on a hydrocarbon pool, in which organic molecules (predominantly polymethylbenzenes) trapped within the zeolite act as co-catalysts. Methylation of the hydrocarbon pool species are key steps in the production of ethylene and propylene. In secondary reactions polycyclic aromatic compounds can be formed. These molecules are considered as coke and lead to catalyst deactivation.

In this contribution the activities of benzene, naphthalene, and phenanthrene toward methylation in H-SSZ-13, H-SAPO-34 and H-ZSM-58 are compared based on theoretical calculations. This allows the assessment of the influence of acid strength on the stability of these species and their tendency to lead to coke formation. Additionally, a possible route for the formation of peri-fused bicyclic compounds via isobutene is proposed in an effort to investigate its contribution to the formation of coke. Furthermore, calculated IR spectra and experimentally obtained spectra are compared.