CATL: Division of Catalysis Science and Technology

62 - Advanced molecular simulations of elementary steps in zeolite catalysis under reaction conditions

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Abstract:Zeolites are prominent heterogeneous catalysts with numerous applications in today's chemical industry. The number of zeolite structures and their applications still increases in view of the shift to alternative feedstocks. Nonetheless, many features of zeolite catalysis are only superficially understood. In that respect many computational chemistry methods are actively used in the field of zeolite catalysis and recent developments enabled the application of advanced molecular dynamics (MD) techniques.[1] Such approach allows describing the impact of catalyst and process related parameters, such as feed composition, reaction temperature, catalyst topology and Brønsted acidity (Figure 1), as shown in this contribution.

As a case study, benzene and propene methylations are considered as they are model compounds for the hydrocarbon pool species acting as co-catalysts during methanol conversion to hydrocarbons.[2] It has been reported that these reactions either occur in a concerted or stepwise fashion and that the competition between these mechanisms can be driven by the aforementioned factors.[3,4] In our MD study, we assess the impact of four factors on the reaction mechanism and kinetics. By varying the temperature and number of methanol and water molecules in the system, the influence of feed composition and temperature are assessed. Furthermore, we evaluate the influence of zeolite topology and acidity by comparing results for the AFI-structured H-SSZ-24 and TON-structured H-ZSM-22 materials. This study shows the strength of an MD-based approach when modeling zeolite-catalyzed reactions under true reaction conditions.

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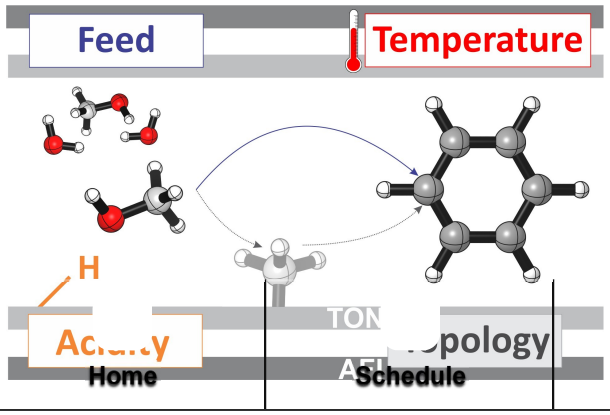

Figure 1. Overview of catalyst and process related factors included in our study.