Molecular modeling within zeolite catalysis :
Examples from the Methanol-to-Olefin process and olefin cracking

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Zeolites are amongst the most widely investigated and topical inorganic materials. They are widely used in industry for a plethora of applications. Within this contribution we specifically highlight the role molecular modeling can play within **zeolite catalysis**.[1] Molecular modeling in close synergy with experimentalists is crucial in understanding the function and nature of the active site and may help to understand the nature of reactive intermediates. However modeling efforts need to account for **realistic working conditions** such as the true nature of the feedstock, framework flexibility, temperature and pressure effects, competitive pathways,… Our approach consists in simulating complex chemical transformations in nanoporous materials using first principle molecular dynamics methods at real operating conditions, capturing the full complexity of the free energy surface.[2] The approach is illustrated for two industrially important processes: **the methanol to olefin process and catalytic cracking of olefins**.[3] For the MTO reaction, we illustrate how the subtle interplay between various factors may lead to catalysts with longer lifetime and/or better selectivity towards the desired olefins. The role of zeolite acidity, feed composition, temperature, and post-synthetic modification on the product distribution will be discussed.[4, 5] For catalytic alkene cracking, we show how advanced molecular dynamics simulations at true operating conditions, may reveal the nature of the intermediates (alkoxides, π-complexes, carbenium ions) and the dominant cracking pathways.[6] Throughout the talk we show the importance of modeling techniques that account for realistic working conditions. The approach followed here may greatly impact catalysis science and reveal insights that were undiscovered so far.

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