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MOLECULAR MODELING AT OPERATING CONDITIONS FOR ZEOLITE CATALYZED HYDROCARBON CONVERSIONS

CHEMISTRY FOR THE ENVIRONMENT
4. Catalysis, Sorption and Separation for a Cleaner Environment

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Abstract

The last decennia, major efforts have been performed to induce the transformation of an oil based economy to the usage of alternative feedstocks to produce chemicals. This effort goes hand in hand with the development of cleaner processes to meet the mounting environmental concerns. The design of innovative and efficient catalysts for hydrocarbon conversion is of utmost importance to facilitate the transition to more sustainable chemical processes. Within this contribution we focus on two important processes in the field of zeolite catalysis, namely catalytic alkene cracking and methanol-to-olefins, which have the potential to play a crucial role in closing the carbon loop, via the (direct) transformation of CO2 into fuels, aromatics or olefins. [1, 2]

Zeolites are widely used in industry for a plethora of applications.[3] However, in general the catalysis function is very complex and it is very difficult to obtain insight into the reaction mechanism solely based on experiments. Therefore, **molecular modeling, in close synergy with experimental studies,** is crucial to understand the complexity of the catalyst and design new catalysts, which show an improved lifetime and a high selectivity towards the targeted products.

In this talk, we emphasize the importance of accounting for **realistic working conditions to unravel the true nature of the intermediates and the prevailing reaction routes**. Our approach consists in simulating complex chemical transformations in nanoporous materials using **first principle molecular dynamics methods at operating conditions, capturing the full complexity of the free energy surface**.[4] Where possible our theoretical data is linked with spectroscopic data. The approach followed here may greatly impact catalysis science and reveal insights that were undiscovered so far.

Acknowledgement VVS acknowledges the European Union's Horizon 2020 research and innovation programme (consolidator ERC grant agreement No 647755 – DYNPOR (2015-2020)).

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