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High throughput in silico screening for tailored catalytic reactivity and selectivity

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First-principles simulation has become a reliable tool for the prediction of structures, chemical mechanisms, and reaction energetics for the fundamental steps in homogeneous and heterogeneous catalysis. Details of reaction coordinates for competing pathways can be elucidated to provide the fundamental understanding of observed catalytic activity, selectivity, and specificity. Such predictive capability raises the possibility for computational discovery and design of new catalysts with enhanced properties.

In the case of mesoporous materials like zeolites, the well-defined pore structures and adjustable reactivity centers in the pore walls allow for efficient control of the catalytic properties. In addition to the reactivity at the catalytic center, the mobility of the reaction components throughout the network structure is crucial to the design. In this contribution we will use GPU-accelerated molecular dynamics simulations to study the diffusion of small molecules through zeolite structures.

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