Molecular dynamics study of diffusion in 8-ring acidic zeolites

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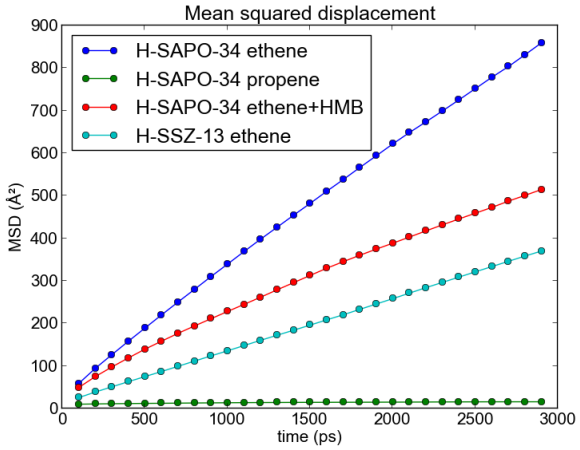
Acidic zeolites are efficient catalysts in the methanol-to-olefin (MTO) process [1]. Currently, research is often focused on tailoring zeolites toward product selectivity and resilience to inactivation by coke formation. One of the key factors that determine product selectivity is the size of the pores, which limits the size of the MTO intermediates and of the products that can diffuse through the zeolite channels. It has been shown that in H-SAPO-34, an extensively studied 8-ring zeotype catalyst, increase in ethene selectivity with time on stream is due to product shape selectivity, which changes with the degree of pore clogging [3].



We use molecular dynamics simulations to model the diffusional properties of ethene and propene, two major products of the MTO process, in 8-ring acidic zeolites during different stages of the MTO process. The diffusion process can be described by discrete hopping events between the cages through the 8-ring windows. While ethene diffuses freely across the porous networks, the mobility of propene is severely hampered. Moreover, the presence of MTO intermediates inside the cages significantly affects the diffusivity of the small molecules. Furthermore, the diffusion constant depends strongly on the framework type, flexibility and chemical composition.

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