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Poster abstract

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Title: Ab initio molecular dynamics study on the influence of water on methanol conversion in H-SAPO-34

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Summary (max 200 words)**:**

Due to growing relevance of renewable resources, interest in the methanol-to-olefin (MTO) process has grown for the production of light olefins. Studies on the reaction mechanism governing this process have been ongoing for years. Nowadays, mechanisms based on hydrocarbon pool (HP) species co-catalyzing the reactions have been generally accepted for the MTO process. For H-SAPO-34, an important industrial catalyst for this process due to its high selectivity to light olefins, two main mechanisms based on hexamethylbenzene as a HP species have been proposed for the production of olefins, namely the paring and side-chain mechanism. Water has an important influence on the MTO process, since it is a byproduct of both the methanol synthesis and the MTO process. Furthermore, addition of water to the methanol feed is known to reduce the coking rate and maximize selectivity to light olefins. For this poster, the influence of water on the framework flexibility, proton mobility and stability of the aromatic intermediates of the side-chain mechanism is investigated in H-SAPO-34 by means of ab initio molecular dynamics simulations. Furthermore, the dependence of the free energy barrier of the reactions of the side-chain cycle on the water loading is investigated via metadynamics simulations.