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**INVESTIGATION OF CONFINEMENT EFFECTS ON ZEOLITE-  
CATALYZED METHYLATION REACTIONS**

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Catalytic conversion of methanol to light olefins (MTO) over acidic zeolites is currently one of the most prominent alternatives to traditional crude oil cracking processes for the production of ethene and propene. The underlying reaction mechanisms have been under debate for decades, with current insight strongly supporting an indirect mechanism based on the hydrocarbon pool hypothesis: olefin formation is found to occur through repeated methylation and subsequent elimination and/or cracking reactions of organic co-catalysts inside the zeolite pores.[1] Depending on the characteristics of the zeolite material, the predominant hydrocarbon pool species vary from smaller alkenes to bulky polymethylbenzenes.[2] Theoretical studies showed that methylations are generally the rate-determining steps in the olefin producing catalytic cycles; therefore it is of utmost importance to gain an in-depth understanding of these reactions.[3,4]

Quantum chemical calculations on extended cluster models that mimic the local environment of the active site were used in this work to model methylation reactions in a selection of zeolite frameworks. Activation barriers and rate constants are then mutually compared to assess the influence of confinement effects caused by different catalyst topologies. The balance between accuracy and computational efficiency signifies this approach as an important step toward routine study of reaction steps in heterogeneous catalysis.[5]

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