

Growth of naphthalenic HP species: influence of the CHA topology from a molecular modeling perspective

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The conversion of methanol to olefins (MTO) forms a key process for the production of higher valued products that can easily be transported, such as ethene and propene. Unraveling the underlying reaction mechanism of this complex process has already shown to be very challenging. Recent ab initio calculations, in combination with experimental data, are in strong support of the “hydrocarbon pool (HP) model” as opposed to a direct route [1]. The HP has been described as a catalytic scaffold inside the zeolite building, consisting of polymethylbenzenes and their cationic derivatives. The exact nature and reactivity of the HP species is still unclear, however, and is probably highly dependent on zeolite topology.

Within this contribution, the growth of naphthalenic species through successive methylations are studied in the SSZ-13 catalyst from a theoretical viewpoint [2]. The influence of space limitations imposed by the zeolite framework is investigated in detail. Reaction rates and kinetic parameters are evaluated based on energies and frequencies originating from reliable ab initio data. The latter were obtained by taking into account a large portion of the zeolite, as to be representative for the actual topology.

References [1] D. M. McCann, D. Lesthaeghe, P. W. Kletnieks, D. R. Guenther, M. J. Hayman, V. Van Speybroeck, M. Waroquier, J. F. Haw, *Angew. Chem. Int. Ed.* **47**, 5179.(2008); [2] K. Hemelsoet, A. Nollet, M. Vandichel, D. Lesthaeghe, V. Van Speybroeck, M. Waroquier, *ChemCatChem* **1**, 373 (2009).