COMP Emilio Esposito, Michael Feig, Jeffry Madura, Melissa Landon Thursday, March 31, 2011

299 - Kinetic study of methylation reactions in zeolites

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Catalytic methanol-to-olefin conversion (MTO) in acidic zeolites is one of the most prominent alternatives to traditional crude oil cracking processes for the production of light olefins. The underlying reaction mechanisms have been under debate for decades. [1] Theoretical modeling has proven to be an invaluable tool in unraveling the complex reaction network. The current study investigates methylation reactions of hydrocarbons present inside the zeolite pores, which are known to be the rate-determining steps in the MTO process. [2] As it is very difficult to obtain experimental kinetic data on individual reaction steps, there is an ongoing interest in accurate determination of barriers and rate constants using theoretical methods. Quantum chemical calculations on extended cluster models were used in this work to obtain reaction barriers and rate constants that are comparable to experimental data. The balance between accuracy and computational efficiency signifies this approach as an important step toward routine ab initio prediction of rate constants in heterogeneous catalysis.

[1] M. Stocker, Micro. Meso. Mater., 1999, 29 (1-2) pp. 3-48
[2] D. Lesthaeghe, J. Van der Mynsbrugge, M. Vandichel, M. Waroquier, V. Van Speybroeck, ChemCatChem, 2010, in press

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