First principle chemical kinetics in nanoporous materials

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The design of an optimal catalyst for a given process is at the heart of what chemists do, but is in many times more an art than a science. The quest for molecular control of any, either existing or new, production process is one of the great challenges nowadays. The need for accurate rate constants is crucial to fulfil this task. Molecular modelling has become a ubiquitous tool in many fields of science and engineering, but still the calculation of reaction rates in nanoporous materials is hardly performed due to major methodological bottlenecks.
In this talk several methodologies are discussed to determine chemical kinetics of catalytic reactions taking place in nanoporous materials from first principles. The discussed items include :
(i) accurate reaction barriers that take into account long range host/guest interactions and
(ii) the preexponential factor within a harmonic and anharmonic description, using cluster and periodic models and by means of static and dynamic approaches.
Two types of industrially important nanoporous materials are considered: zeotype materials including the standard alumino-silicates but also related alumino-phosphates and the fairly new Metal-Organic Frameworks (MOFs). For the zeotype materials, reactions taking place during the Methanol-to-Olefin process (MTO) are chosen. A typical MTO catalyst is composed as an inorganic cage with essential organic compounds interacting as a supramolecular catalyst. For the hybrid materials, firstly accurate interaction energies between xylene based isomers and MOF framework, will be determined.