CBI ERLANGEN

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Multiscale modeling of heterogeneous reactions: From the active center to the reactor

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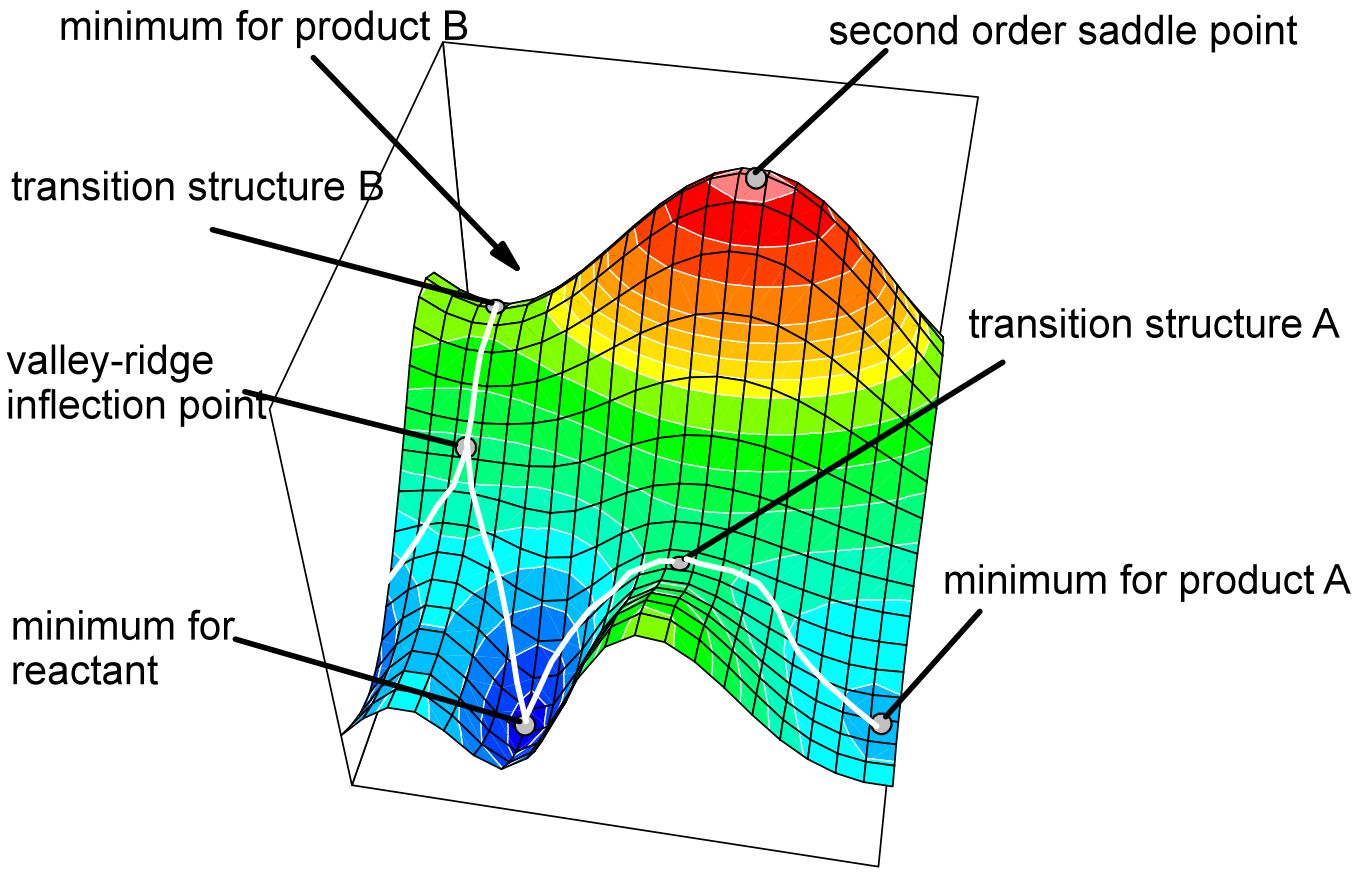

A hierarchical multiscale approach will be presented to calculate effective rates of reaction for a zeolite catalysed reaction system. The first step in this approach involves the determination of intrinsic rate coefficients for all elementary reactions by means of quantum chemical calculations on various levels of accuracy combined with transition state theory. The second step are the calculations of multicomponent adsorption isotherms and diffusion coefficients of all species by means of Monte Carlo and Molecular Dynamics simulations. The ideal Adsorption Solution Theory (IAST) and the Stefan-Maxwell approach can be used in many cases for simulating multicomponent adsorption and diffusion, respectively, whereby data from molecular simulations are used as an input. The third step comprises a continuum description of a zeolite crystal based on a macroscopic reaction-diffusion equation which employs input data from the quantum chemical calculations and molecular simulations. A fourth step involves fixed bed reactor simulations based on the continuum description of single zeolite crystals.

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