# New Routes for Production of Fuels and Chemicals: From Molecular Modeling to Reactor Optimization

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**Abstract:** The lecture will focus on new routes for the production of fuels and chemicals by heterogeneously catalyzed gas-phase reactions. Understanding and optimization of heterogeneous reactive systems require the knowledge of the physical and chemical processes on a molecular level. In particular, at short contact times and high temperatures, at which reactions occur on the catalyst and in the gas-phase, the interaction of transport and chemistry becomes important. Transient processes, temporally and spatially varying inlet and boundary conditions will complicate the understanding of the reactor behavior. The overall reaction rate may be limited by chemical kinetics, transport of species to the catalytic surface from the gaseous flow, diffusion in a porous catalyst structure, or by the spatial and temporal temperature distribution.

It will be shown how the understanding of the chemical and physical processes on a molecular supports the design and optimization of chemical reactors and processes following an approach of hierarchical models reaching from quantum mechanical simulation via Monte Carlo simulations to Computational Fluid Dynamics. Furthermore, the coupling of two- and three-dimensional reactive flows including complex chemical reaction networks with mathematical optimization algorithm and their benefit for the solution of reaction engineering problems will be discussed.

Applications will cover synthesis of basic chemicals and hydrogen from fossil and renewable fuels, and high-temperature fuel cells.

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