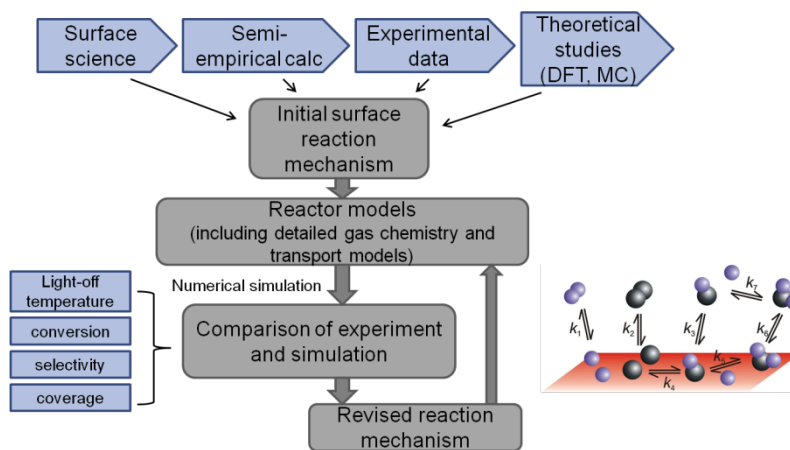


Catalytic conversion over platinum

Background: Reforming and partial oxidation of hydrocarbons, combustion of natural gas, and the reduction of pollutant emissions are important examples for catalytic reactions over platinum. For a better understanding of the kinetics of the elementary-step reactions on platinum coated catalysts, detailed modeling and simulation techniques are useful.



Scheme of the development of a heterogeneous reaction mechanism

Project: Our research is to set up a reliable unified surface mechanism of oxidative conversion of light hydrocarbons over platinum. We first established several sub-mechanisms (H_2/O_2 , CO/O_2 , CH_4/O_2) applicable for a wide range of temperature and C/H/O ratios. Coupling of these mechanisms leads to an initial mechanism of light hydrocarbons. We expanded this mechanism by important side reactions and by coverage dependencies of activation energies. According to this step-by-step procedure, a detailed C1-mechanism is developed.

The mechanism is evaluated against own experimental measurements at different reactor configurations and literature data on partial oxidation and steam/dry reforming reactions. Furthermore, the mechanism is examined for different catalysts with varying Pt loading and for different gas compositions. The mechanism is also ensured to be thermodynamically consistent.

There is an industrial interest to develop and design new catalyst and process options for dry reforming of CH_4 (see: High-temperature catalysis – dry reforming of methane). The detailed C1-mechanism also describes this industrially used Pt-based catalyst.

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