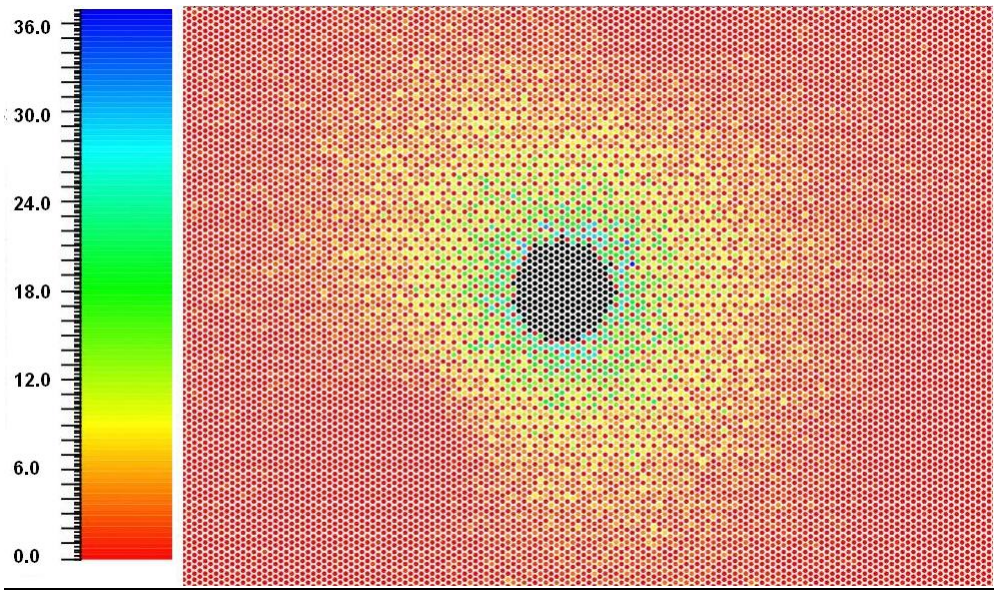
Kinetic Monte Carlo Simulations of catalytic reactions with MoCKa

Background: Over the last years kinetic Monte Carlo Simulations have become important tools for the theoretical investigation of surface processes. Especially in heterogeneous catalysis, where there is an increased demand for more efficient catalysts, kinetic Monte Carlo methods can contribute to understanding the molecular processes underlying the macroscopic phenomena. With these insights, optimization of existing and design of new catalysts should become possible.



Capture zone of one platinum particle (black) with the number of desorptions per lattice site (circles) from none (red) to 36 (blue) during the whole simulation

Project: The program MoCKa enables us to examine almost every catalytic system, but so far we focused on systems with nanoparticles scattered on a support material, where so-called spillover or reverse spillover processes occur. Generally these processes can be described as the mobility of an adsorbed species from one phase with a low adsorption barrier (donor) to one phase with a high adsorption barrier (acceptor). The process with a nanoparticle as donor is called spillover, whereas the process with a nanoparticle as acceptor is called reverse spillover. Through these processes a seemingly inactive material can become catalytically active. Kinetic Monte Carlo methods are used to simulate a chronologically correct sequence of surface configurations with the help of random numbers. They provide information about the correlation between particle characteristics (such as radius, number and distance) and catalytic performance. Additionally, so-called spillover areas (capture zones for reverse spillover) can be obtained by MoCKa's postprocessing tools, where the number of adsorptions (desorptions for reverse spillover) per lattice site is counted and then visualized. From this, one can gain information about the optimal particle distance. The efficient *Variable Step Size Method* (VSSM), where the process in each step is chosen randomly from a list of all possible processes, is used in our simulations, but the *First Reaction Method* (FRM) is also available in MoCKa. In the future, the focus will be shifted to 3D-kinetic Monte Carlo simulations, e.g. diffusion of H_2 into palladium or catalytic reduction of NO on platinum.

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Selected publications: O. Deutschmann (Ed.), Modeling and Simulation of Heterogeneous Catalytic Reactions: From the Molecular Process to the Technical System, Wiley-VCH (2011); http://kmc-simulations.org; F. Kuhn, L. Kunz, O. Deutschmann, J. Catal. (2012).