Master Thesis Project

Developing parallization methods for kinetic Monte Carlo simulations

This aim of the project is to develop Python-based parallelization methods to enhance the capability of kinetic Monte Carlo simulations.

Catalysis is an enabling technology that is used to produce chemicals, green-fuels and clean exhaust streems. One trend in computational catalysis is to build models based on only quantum mechanics and thermodynamics. Such models are used to explore how materials choices and operating conditions affect the catalytic reactions. Chemical reactions occure typically on different timescales making their overall dynamic simulations challenging. Simulating catalytic reactions with kinetic Monte Carlo methods have the advantage that details in the surface structure can be incorporated. The Monte Carlo approach represents also a challenge when simulating large or complex systems. However, because of the independence of reaction steps on different parts of the system, we see a large potential to overcome such bottlenecks by using parallelization methods.


Hebbe-Computercluster

Python libraries offer various different possibilities of parallelizing using either OpenMP or MPI. In addition, Python allows for the incorporation of other languages such as Fortran or C/C++ for further developments. In the master thesis project, general parallelization methods shall be incorporated and evaluated for an existing kinetic Monte Carlo code. High performance computers can be used for testing purposes.

The work will include mainly programming using Python and eventually other languages as Fortran or C/C++. The developed parallelization methods shall be incorporated into the MonteCoffee kinetic Monte Carlo code.

Contact Dr. Elisabeth Dietze (dietze@chalmers.se) or Prof. Henrik Grönbeck (ghj@chalmers.se) to find out more about the project.