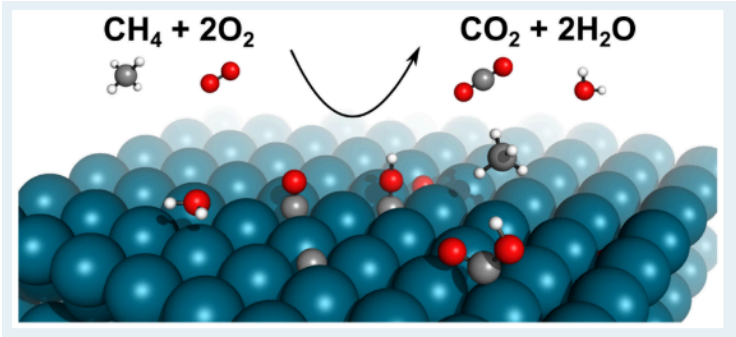
Master Thesis Project

Quantum mechanical descriptions of chemical reactions

This project will develop a model that can describe a technological important chemical reaction directly from quantum mechanics and thermodynamics.



The greenhouse gas potential for global warming of methane exceeds that of CO_2. Therefore, it is desirable to minimize methane emissions by oxidizing preferably to CH_3OH or alternatively to CO_2 and H_2O. The catalytic reaction is done usually over Pd or Pt based catalysts where Pd is most active in oxygen rich environments. A current research question is whether metallic Pd or oxidized PdO constitute the most active phase of the catalyst. The Master Thesis project targets this challenge.

The project will develop a model to describe methane oxidation using quantum mechanics and thermodynamics. The project is a part of a larger effort within the division to describe the reaction and will concentrate on developing models for adsorbate-adsorbate interactions. Adsorbate-adsorbate interactions often lead to crucial changes in adsorption properties, which influence the overall catalytic activity.

It is generally difficult to include adsorbate-adsorbate interactions in models because of the complexity with many adsorbates and structural configurations. Here we suggest developing cluster expansions for the different types of interactions.

The work will include quantum mechanical calculations using the program VASP and programming using Python. The resulting interaction model shall be incorporated into a kinetic Monte Carlo model.

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