In pursuit of a 95% reduction in CO2 emissions, the development of CO2-based higher alcohols as alternative fuels is paramount for the future of the mobility sector. These innovative fuels, acting as sustainable substitutes for traditional gasoline and diesel. In this context heterogeneous catalysts with the NixPt1-x composition have demonstrated remarkable activity and stability in synthesizing isobutanol. Notably, the catalyst’s surface-related activity exhibits a non-linear dependency on the alloy composition, accompanied by pronounced deactivation with higher Pt content. However, the precise chemical active sites governing the reaction steps remain elusive. The focus of this thesis is to ascertain the thermodynamically stable configurations of the metal alloy formed. This thesis represents a collaborative effort between the Institute of Energy and Climate Research - Electrochemical Process Engineering (IEK-14) at Forschungszentrum Jülich and the Junior Professorship for Multi-Scale Modeling of Heterogeneous Catalysis in Energy Systems (MODES) at RWTH (https://www.modes.rwth-aachen.de). The research will be conducted at MODES laboratories.

We are offering a

**Master Thesis - Monte Carlo Simulations of NixPt1-x Dilute Alloy Surfaces**

**Your Job:**
You will focus on investigating the influence of alloy compositions within a broad range. Monte Carlo Simulations will be executed based on precalculated DFT clusters. Particular emphasis will be placed on discerning the resulting surface and bulk composition of the alloys in correlation to their overall Pt content.

- Careful reading and analysis of assigned literature, as well as basic review of thermodynamics
- Analysis of DFT simulation data on NixPt1-x dilute alloys already calculated at MODES

The job will be advertised until the position has been successfully filled. You should therefore submit your application as soon as possible. We look forward to receiving your application via our Online-Recruitment-System!

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• Learning and performing DFT simulations on NixPt1-x dilute alloys under solvation conditions
• Building a Cluster Expansion model and performing Monte Carlo Simulations to predict stable surface structures
• Using stable structures to calculate adsorption energies for different reaction intermediates and to rationalize experimental results

**Your Profile:**
• Strong performance in your master studies in chemistry or a related field
• Strong command over basic python/C/C++ programming
• Preliminary experience in computational chemistry methods is not a requirement, but very beneficial
• Knowledge in catalysis or surface chemistry is advantageous
• Demonstrated ability to work independently and analytically
• Proficiency in both written and spoken German and English

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