



In Silico analysis of binding nature of different types of Nafion polymer to the catalyst in CCL of PEMFC

Project Description

To enhance the power density and operational efficiency of Polymer Electrolyte Membrane Fuel Cells (PEMFCs), which is crucial for their broader commercialization, a deep understanding of the nanostructure dynamics within the cathode catalyst layer (CCL) is essential. The CCL's performance is significantly influenced by the interactions between its components, notably the ionomer and catalysts. This project targets these interactions by examining the binding free energy between different Nafion ionomers and a variety of catalyst materials using Molecular Dynamics (MD) simulations. Improved binding energy is hypothesized to enhance catalyst utilization, increase mechanical stability, and superior ionic conductivity.

The primary objective is to analyze and optimize the binding interactions between Nafion ionomers of different equivalent weights and catalysts. Using the GROMACS (Groningen Machine for Chemical Simulations) software, a detailed investigation will be conducted to calculate the binding free energies under different operational aviation scenarios. This will include variations in pressure, Sulfur content in Ionomer and stoichiometric conditions.

Requirements

- master degree in mechanical, chemical, process engineering or related disciplines
- excellent knowledge in molecular dynamics simulations
- experience in using the MD simulator GROMACS
- very good skills in English

Contact information

Applications should be sent by e-mail to Prof. Dr.-Ing. Gabriele Raabe: **G.Raabe@tu-braunschweig.de**

The entry date is as soon as possible, and the duration of employment is limited to 6 months. The position is part-time with 50% of the regular weekly working time (currently 19,9h). Ongoing applications are possible until all positions are filled.

The payment is made according to task assignment and fulfillment of personal requirements to salary group EG 13 TV-L. International applicants may have to successfully complete a visa process before hiring can take place. Candidates with handicaps will be preferred if equally qualified. Please enclose a proof. The position is part of the SE²A International Female Program, so only applications by female graduates of non-German universities are possible.

All documents should be in PDF format, preferably in a single file. Personal data and documents relating to the application process will be stored electronically. Please note that application costs cannot be refunded.