ReaxFF simulations on the reduction of furfural and 5-HMF

Project Description

The project "Fundamentals of ElectroFuel Synthesis for Aviation" is an interdisciplinary approach - combining experimental and molecular dynamics studies - aimed at laying the groundwork of electrochemical synthesis for the systematic and tailored generation of liquid aviation fuels. Therein, the objective of the MD studies is the identification of relevant molecular determinants and interaction patterns of the core electrochemical synthesis process.

In the first project phase, MD simulations using the classical OPLS-AA force field are employed to gain insight into the relevant influencing factors such as microstructural properties, diffusivities etc., which affect the occurrence and kinetics of the reactions, and with this, the selectivity and yield of the synthesis. In the next project phase, also the chemical reactions at the electrode themselves shall be studied using the reactive force field ReaxFF.

In this proposed project, parametrizations of the ReaxFF model available in literature shall be evaluated regarding their ability to correctly reproduce the reduction of furfural and 5-HMF as model reaction.

Requirements

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

Contact information

Applications should be sent by e-mail to PD Dr.-Ing. Gabriele Raabe: **G.Raabe@tu-bs.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 Programme, 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.