PhD-Researcher Position (m/f/d) within the SE²A Research Cluster

Design and (nano)engineering of PEMFC cathode catalyst layers to boost the efficiency and life-time under aviation conditions – MD simulations at the catalyst – ionomer interface

Temporary Position (up to 3 years), up to Salary Level EG 13 TV-L, 100%

Background:

The Cluster of Excellence *SE²A - Sustainable and Energy-Efficient Aviation* is a DFG-funded interdisciplinary research center investigating technologies for a sustainable and eco-friendly air transport system. Scientists from aerospace, electrical, energy and chemical engineering as well as economics and social science are working on the reduction of drag, emissions and noise, life-cycle concepts for airframes, improvements in air traffic management and new technologies for energy storage and conversion. Technische Universität (TU) Braunschweig, the German Aerospace Center (DLR), Leibniz University Hannover (LUH), the Braunschweig University of Art (HBK) and the National Metrology Institute of Germany (PTB) have joined forces in this extraordinary scientific undertaking. The overall project is structured into the three core research areas "Assessment of the Air Transport System", "Flight Physics and Vehicle Systems" and "Energy Storage & Conversion".

(www.tu-braunschweig.de/en/se2a)

The project "Design and (nano)engineering of PEMFC cathode catalyst layers to boost the efficiency and life-time under aviation conditions" is aimed at a systematic study of the relevant key parameters on the O_2 permeation and diffusivity through the ionomer film to the catalytically active Pt-Co and Pt-Ni surface in polymer electrolyte membrane fuel cells (PEMFCs). It the subproject in the group of Gabriele Raabe, molecular dynamics simulations will pe performed to illuminate the underlying molecular processes at the catalyst – ionomer interface that dominate the O_2 transport resistance. Detailed atomistic molecular simulations with optimized molecular models will be employed to identify the critical parameters on the local O_2 transport in the cathode CL. The project is an interdisciplinary approach, in which the key findings from the MD studies will be brought together with experimental results from the group of Mehtap Oezalsan (Institute of Technical Chemistry) for a joint assessment and analysis to deduce information on both optimal ionomer and catalyst compositions as well as on most suitable operation conditions to minimize the O_2 transport resistance for cathode CL with alloyed Pt-Ni/Co catalysts**.** Therefore, the research within this subproject will be carried out in close collaboration with the PhD researcher in Mehtap Oezaslan's group.

Employment:

The position is located at the Institute of Thermodynamics (http://ift-bs.de/) at TU Braunschweig. The entry date is as soon as possible, and the duration is initially limited until the end of 2025. The position is part-time suitable, but should be occupied 100%. For all doctoral researchers of the cluster, an active

participation in SE²A's own qualification programme is mandatory, the time effort for this training measure entails 10% of the working time. The payment is made according to task assignment and fulfillment of personal requirements up to salary group EG 13 TV-L. International applicants may have to successfully complete a visa process before hiring can take place. Applications from international scientist are welcome. The Cluster SE²A aims to increase the share of women in academic positions. Applications from female candidates are very welcome. Where candidates have equal qualifications, preference will be given to female applicants. Candidates with handicaps will be preferred if equally qualified. Please enclose a proof.

Task:

- Development of optimized interface force fields for the ionomer, water and oxygen interaction with the Pt-Ni and Pt-Co surface – based on QM simulations, employing an inhouse genetic algorithm
- MD studies on the morphology of PFSA ionomers on different Pt-Ni(111) and Pt-Co(111) slaps
- Analysis of the O_2 permeation through the thin ionomer layer by MD simulations.
- Contribution to the teaching activities of Gabriele Raabe's group in different Master's courses

Who we are looking for:

- a highly motivated candidate with a master degree in mechanical, chemical, process engineering or related disciplines, with
- knowledge/experience in molecular dynamics simulations
- ideally also knowledge/experience in quantum mechanical simulations
- good programming skills
- excellent oral and writing skills in English (language skills in German are beneficial)
- self-initiative and a result-orientated working approach

Application Process:

Applications should be sent by e-mail to **G.Raabe@tu-braunschweig.de** and must contain the following documents Motivation Letter

- Curriculum Vitae including complete address, phone number, email address, educational background, language skills, and work experience
- Copies of bachelor and master diploma and transcript of grades in original language and in English or German translation
- Additional Documents must be provided on request

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. For the purpose of carrying out the application process, personal data will be stored.

For more information, please call Gabriele Raabe on +49 (0) 531 391-2628 or contact her via e-mail.