DIFFER (Dutch Institute for Fundamental Energy Research) and Technical University of Eindhoven, the Netherlands, are looking for a

PhD on Microkinetic Modeling for Water Splitting

Description and scientific aim

Electrochemical materials and interfaces are present in many energy systems, such as fuel cells, batteries, or water splitting devices. The performance of such devices is strongly related to the materials and interface properties. Therefore, understanding and tuning of these properties are crucial in order to reach highest performance and to supply alternative, sustainable energy solutions for the future.

In this frame, we recently received a grant for two PhD students, one on experiments and one on modeling. The scientific aim of this grant is to identify the limitations at photoelectrochemical water splitting interfaces by intertwining operando spectroscopy with microkinetic modeling.

The current vacancy is for the modeling PhD. You will work on microkinetic modeling using methods of control. Close collaboration with the experimental PhD student who focuses on operando spectroscopy, is planned.

You will be hired at TU/e and will be embedded both in the group "Control Systems (CS)" of the Department of Electrical Engineering at TU/e as well as in the group "Electrochemical Materials and Interfaces (EMI)" at DIFFER. You will have a working places in both groups, both located on the campus of Tu/e. In the CS group, we focus on dynamic modeling and model-based control of complex dynamic systems. The vision is to apply and develop novel techniques and methods for the modeling, automated control and optimization of dynamical systems so as to influence their behavior towards desired specification of performance, safety, efficiency, product quality and improved environmental conditions. In the EMI group, we focus on microkinetic modeling and operando spectroscopy of (photo-)electrochemical systems.

Responsibilities and tasks:

- build microkinetic models for water splitting including (non)linear optimization schemes to translate impedance spectra in physico-chemical quantities
- simulate electrochemical data and validate models using system identification techniques
- extend your models to estimate experimental data
- identify the limiting processes at the interface in collaboration together with the experimental PhD student in the project
- collaborate with researchers from the CS group and/or other scientific groups to discuss your research and to broaden and deepen your knowledge and expertise
- connect your data to ML and AI databases
- involve students in your project and supervise them (Master, Bachelor, interns)
- disseminate your research output at conferences and with scientific papers
- contribute actively to a vivid research environment at TU/e and at DIFFER

Qualifications:

We seek an enthusiastic and talented control or system identification engineer with experience or at least affinity to chemistry. Alternatively, you can also have a background in chemical modeling, microkinetic modeling, or (theoretical) physical chemistry / electrochemistry with affinity to modeling and simulations; knowledge in electrochemical methods is desired. You are expected to work closely together with the experimental PhD student of the project which will be hired at DIFFER. We therefore look for an excellent team player with superb communication skills and motivation to discuss science in a highly multidisciplinary field. Good verbal and written communication skills in English is a prerequisite in our international and interdisciplinary team.

Further information:

DIFFER and TU/e strive to achieve a diverse workforce to develop talent and creativity by bringing together different perspectives. As such we encourages applications from minorities. Further information on the vacancy is available through <u>TU/e webpage</u> or via the leader of the Control Systems group at Electrical Engineering, TU/e, Prof. Siep Weiland, Tel: +31 (0) 40 247 5979, e-mail: <u>s.weiland@tue.nl</u> OR of the Electrochemical Materials and Interfaces group, DIFFER, Dr. Anja Bieberle, Tel: +31 (0) 40 3334 801, e-mail: <u>a.bieberle@differ.nl</u>

Application procedure:

We invite you to submit a complete application by using the 'apply now'-button on the TU/e webpage: <u>TU/e webpage</u>.