PREDICTOR

JOB POSTING

Recruiting organisation
Zürcher Hochschule für Angewandte Wissenschaft ZHAW

Subproject title
Electrochemical double layer and meso-scale modelling

Starting date
1st April 2025 (or earlier if preferred)

Salary
The Doctoral Network "PREDICTOR" is financed by the European Union under the framework of the program HORIZON Europe, Marie Skłodowska-Curie Actions. The doctoral candidate will be hired for 36 months under contract by ZHAW.

Background information
Marie Skłodowska-Curie Doctoral Networks are joint research and training projects funded by the European Union. Funding is provided for doctoral candidates from both inside and outside Europe to carry out individual project work in a European country other than their own. The training network "PREDICTOR" is made up of 22 partners, coordinated by Fraunhofer ICT in Germany. The network will recruit a total of 17 doctoral candidates for project work lasting for 36 months.

PREDICTOR aims to establish a rapid, high-throughput method to identify and develop materials for electrochemical energy storage. It will enable the rapid identification, synthesis and characterization of materials within a coherent development chain, replacing conventional trial-and-error developments. To validate the PREDICTOR system, the case study will be active materials and electrolytes for redox-flow batteries. Within the project, three demonstrator battery cells (TRL3-4) will be assembled and tested with the newly developed materials.

Our objectives:
- A **modelling and simulation tool** for the computational screening of organic chemicals based on their potential performance in energy storage systems.
- **Automated** chemical synthesis, electrolyte production and characterization methods, so that the chemicals identified in the screening step can be rapidly produced and tested for their suitability in energy storage applications.
- **Artificial- intelligence- based** self-optimization methods that allow experimental data from material characterization to be fed back into automated experimental methods to enable self-driving laboratory platforms and for modelling and simulation tools, improving their accuracy.
- **Data management systems** to standardize and store the data generated for further use in model validation and self-optimization processes.

Job description
The advertized subproject forms part of the Marie Skłodowska-Curie European Training Network „PREDICTOR", and is fully funded by the Swiss State Secretariat for Education, Research and Innovation SERI. It will be carried out by one doctoral candidate at the Institute of Computational Physics at ZHAW (PhD supervision at CNRS in France) over a period of 36 months.

With over 11,000 students and around 3,000 employees, the ZHAW Zurich University of Applied Sciences is one of the largest multidisciplinary universities of applied sciences in Switzerland.

As one of the leading technical universities in Switzerland, the School of Engineering (SoE) focuses on future-oriented topics. 13 institutes and centres guarantee high-quality education as well as research and development with a focus on energy, mobility and health.

At the Institute of Computational Physics (ICP), physicists, mathematicians and engineers work on applying methods and results from basic research to industrial problems. For more than 20 years, the ICP has been developing multiphysics computer models for industrial applications (e.g. in the field of hydrogen technology, photovoltaics or coupled-physics modelling). Together with its partners from science and industry, the ICP develops solutions in applied research and development.

The goal of this doctoral thesis is to develop scale-specific models to be included in a multi-scale framework for computational high-throughput screening of organic redox pairs. The recruited researcher will develop new models for the electrochemical double layer that capture important surface processes, including surface coverages of adsorbed species and multi-step reactions. In a

PREDICTOR

JOB POSTING

second step, the formulated double layer model will be integrated into a pore-scale model describing the transport of mass, momentum, and charge through a porous electrode. The pore-scale model will be used to identify limiting factors of the electrochemical conversion and evaluate effective transport properties, including diffusion coefficients and effective reaction rates, which can be used in macrohomogeneous cell models. The developed models will be integrated into the multi-scale modelling framework in collaboration with other doctoral students.

Benefits

The recruited researcher will have the opportunity to work as part of an international, interdisciplinary team of 17 doctoral candidates, based at universities and industrial firms throughout Europe. She/he will be supported by two mentors within the PREDICTOR project, and will have multiple opportunities to participate in professional and personal development training. Through her/his work she/he will gain a unique skill-set at the interface between modelling and simulation, high-throughput experimentation / characterization and self-optimization and data management over different length scales from nano to the macroscopic level.

She/he is expected to finish the project with a PhD thesis and to disseminate the results through patents (if applicable), publications in peer-reviewed journals and presentations at international conferences.

Requirements

Qualifications/experience:

- In accordance with the European Union's funding rules for doctoral networks, applicants must NOT yet have a PhD
- Excellent master's degree in computational science, physics, mathematics, engineering, or a related discipline
- Familiarity with mathematical modelling and numerical methods for ordinary and partial differential equations
- Experience in modelling and simulation of physical- and/or chemical- processes
- Strong interest in working in a cross-disciplinary, collaborative project at the interface of electrochemistry and mathematical modelling
- Experience in at least one programming language for scientific computing (C/C++, Matlab, Fortran, Python, Julia, …)
- Good communication skills and willingness to work in collaborative projects with multiple partners and present results at conferences, project meetings and partners
- Very good English language skills (German is beneficial)
- Self-motivation and the ability to achieve goals independently as well as to contribute effectively to the team

Mobility:

The applicant must not have resided or carried out her/ his main activity (work, studies etc.) in Switzerland for more than 12 months in the past 3 years.

How to apply

Please send your CV by e-mail (preferred) or by post, quoting the reference PREDICTOR-DC14-ZHAW:

predictor-dc14-zhaw@proton.me

Application deadline: 23rd November 2024