PREDICTOR

JOB POSTING

Recruiting organisation
Karlsruhe Institute for Technology (KIT)
Kaiserstraße 12
76131 Karlsruhe
Germany

Subproject title
Model predictive control (MPC) for flow batteries

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 the Karlsruhe Institute of Technology, with a monthly gross salary of app. 3.200,-.

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 candida- tes 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 is fully funded by the Marie Skłodowska-Curie European Training Network "PREDICTOR". It will be carried out by one doctoral candidate at the Institute of Mechanical Process Engineering, PhD supervision under the guidance of Prof. Dr. Hermann Nirschl over a period of 36 months.

The Karlsruhe Institute of Technology (KIT) is "The Research University in the Helmholtz Association." As the only German university of excellence with a national large-scale research sector, we offer our students, researchers, and employees unique learning, teaching, and working conditions.

In previous projects a framework for the simulation-based screening of electroactive materials for aqueous and nonaqueous organic redox flow batteries (RFBs) has been developed. It adopted a multiscale modelling paradigm, in which simulation methods at different physical scales were further advanced and linked by combining physics- and data-based modelling. The next step is the implementation of control concepts for single- and multi-stage processes (process chain). This will involve the automatic adjustment of power behaviour, material properties, compensation of unforeseen disturbances, acceleration of start-up and shut-down, and planning and control of optimal trajectories under consideration of uncertainties and process relevant quality criteria (e.g. energy and raw material efficiency). Nonlinear, optimization based and robust control methods will be applied. This is a new challenge for RFB and the topic for an innovative Ph.D. thesis.

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

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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.

She/he will become a member of staff of the only German University of Excellence that conducts large-scale research on the national level. This includes excellent working conditions in an international environment and an active role in research and academic education for our future. The recruited research will benefit from specific training when starting their job and from a wide range of further qualification offers. Further benefits include flexible working time models (flexitime, work from home), sports and leisure offers, as well as child and holiday care services. We also pay a share of EUR 25/month in the Job Ticket Baden-Württemberg, and offer a large variety of dishes, snacks, and beverages at our canteens.

Requirements

Qualifications/experience:
- In accordance with the European Union's funding rules for doctoral networks, applicants must NOT yet have a PhD
- Very good Master in chemical or mechanical engineering or any other background in simulation technologies
- Solid background in the fundamentals of heat and mass transport and in chemical engineering
- Experience in CFD and/or control simulations and programming
- Curiosity and creativity
- Ability to organize and structure an exploratory project
- Fluency in English (min. C1) and if possible German

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

How to apply
Please send your CV by e-mail (preferred) or by post

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Application deadline: 30th October 2024