

JOB POSTING

Recruiting organisation:

Zürcher Hochschule für Angewandte
Wissenschaft ZHAW

Subproject title:

Mathematical modelling of multi-step reactions
and flow cell simulation

Starting date:

1st September 2023 (or earlier if preferred)

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 "MiEI" is made up of 10 partners, coordinated by Fraunhofer ICT in Germany. The network will recruit a total of 12 doctoral candidates for project work lasting for 36 months.

New industrial production strategies like "production on demand" and "Industry 4.0" are increasing the demand for new digital concepts for the chemical industry that are easily scalable and can work like a construction kit. In addition, the reduction of fossil fuel consumption requires novel synthesis concepts with on-demand capabilities paired with the use of electrical energy as a primary source for chemical processes.

MiEI will address this demand from the chemical industry, combining the advantages of electrochemistry, micro process engineering and flow chemistry. The recruited researchers will explore new models for electrodes and electrochemical flow cells and develop innovative integrated prototype cells using printed circuit board (PCB) technology as a mass-scalable and flexible tool. These cutting-edge technologies will

be applied to promising fine chemical and pharmaceutical synthetic routes, which will be further accompanied by techno-economic evaluation defining new business opportunities. The new MiEI technologies and processes will allow safe, flexible and sustainable synthetic routes for the chemical industry of the future.

Job description:

The advertised subproject forms part of the Marie Skłodowska-Curie European Training Network „MiEI“, 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 Karlsruhe Institute of Technology, Germany) 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.

In the MiEI project our aim is to develop and link different models describing flow cells for electroorganic synthesis on different scales and dimensions. Processes will be modelled over a

wide range of length scales ranging from μm to cm. The recruited researcher will explore electrochemical reactions and develop continuum-scale flow cell models. She/he will be responsible for the model-based analysis of flow cells with respect to conversion efficiency, charge efficiency, and selectivity towards desired products. Investigations will also include microfluidics simulations to consider for surface tension in droplet generation, dispersion and microscale channel flow. The recruited researcher will collaborate with other doctoral candidates in the project to improve constructed flow cells and identify appropriate operating conditions.

Benefits:

The recruited researcher will have the opportunity to work as part of an international, interdisciplinary team of 12 doctoral candidates, based at universities and industrial firms throughout Europe. She/he will be supported by two mentors within the MiEI 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 comprising electrosynthesis, flow chemistry and process analytical technologies, as well as modern control engineering techniques. 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, chemistry, engineering, or a related science
- Familiarity with mathematical modelling and numerical methods for partial differential equations is expected

- Strong interest in modelling and simulation in a cross-disciplinary, collaborative project at the interface of organic chemistry and engineering
- Experience in at least one programming language for scientific computing (C/C++, Matlab, Wolfram Language, Python, Julia, ...)
- Strong interest in computational chemistry and mathematical modelling
- 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 MiEI-11DC-ZHA:

miel-11dc-zha@juergenschumacher.de

Application deadline: 24th March 2023