June 2025

Postdoctoral scholarships in "Simulations and modelling of mixed ionic-electronic conducting polymers" at the Laboratory of Organic Electronics, Linköping University, Sweden

A postdoctoral scholarship in **Simulations and modelling of mixed ionic-electronic conducting polymers** is available at Linköping University, Sweden. The position is based at the Theory and Modelling Group, Laboratory of Organic Electronics (LOE), belonging to the Department of Science and Technology, at the University's Norrköping Campus. The LOE is renowned for its world-leading research on organic electronic and optical materials and devices. Its primary theme involves the coupling of ions and electrons as signal carriers for applications in organic bioelectronics, printed electronics, organic energy, and electrochemical devices, and nanooptics. Currently, the research staff of the Laboratory includes more than 150 researchers (professors, senior and junior scientists and PhD students). LOE is also a partner in the Wallenberg Wood Science Center and the Wallenberg Initiative Materials Science for Sustainability.

Background and duties:
Mixed ionic-electronic conducting polymers (MIECPs) are a class of materials that exhibit both electronic and ionic conductivity. These materials combine the high conductivity with the ability to transport ions within their structure. This simultaneous electronic and ionic conductivity is essential in a wide range of devices, including batteries, fuel cells, supercapacitors, sensors, actuators, organic electrochemical transistors, where both electron and ion charge transport are needed for device functionality and performance.

While these materials are already emerging in commercial applications, their broader adoption is still limited by an incomplete fundamental understanding of key material properties—such as morphology, ion and electron transport and injection, and electrochemical doping mechanisms. The primary goal of this project is to develop multiscale computational models and predictive tools for MIECPs, addressing critical knowledge gaps in their fundamental behavior. This includes detailed investigations of the density of states (DOS) and intrinsic capacitance, as well as machine learning-assisted multiscale mobility simulations and graph-theoretical analyses of morphology and ion and electron transport. Computational methods will primarily include all atomistic and coarse-grained molecular dynamics (MD) simulations, hybrid quantum-mechanical/molecular mechanical (QM/MM) approaches, as well as ML and graph-theoretical approaches.

The theoretical studies will be performed in the Theory and Modelling group under supervision of Prof. Igor Zozoulenko. This is a collaborative project that would require visits to the group of Prof. Maria Sammalkorpi at Aalto University (Finland). A collaboration with Prof. Nicolas Kotov (University of Michigan) on graph-theoretical approaches is expected. The present research project will be performed in collaboration with the experimental groups where the obtained theoretical results will help to understand and guide the material and device design.

Qualifications and requirements to applicants:
- The applicant must have or be about to receive a doctoral degree in a subject relevant to the research project (e.g. material science, physics, chemistry, physical or theoretical chemistry, etc.) and needs to be passionate about research. The applicate must have extensive experience with MD simulations. Problem solving ability and creativity, as well as the ability to work independently are essential. Good skills in programming/scripting are highly desirable.
- scholarship may be granted only to non-Swedish citizens with a PhD or equivalent acquired in another country than Sweden. The applicant could not have been employed by Linköping university previously.

- Applicants should preferably have obtained their PhD no more than three years ago.

Starting date
January 2026 or by agreement.

Appointment and Conditions:
- Appointment is initially for one year with a possibility of an extension for the second year depending on a mutual agreement. The scholarship amounts to SEK29000:-/month (tax-free).
- Economy class travel to/from Sweden will be covered.
- Funding can be available to participate in conferences.
- Note, the scholarship does not give any pension rights, sick or maternity pays and other work-related benefits. If you have questions on the terms, please contact HR at the Department of Science and Technology, hr@itn.liu.se.

Application procedure:
The following documents must be submitted when applying for a scholarship
- Motivation letter (1- 2 pages)
- Curriculum vitae, max 2 pages, including names of at least two references
- List of publications
- Copy of the PhD diploma

The application, as a single pdf-file, should be sent electronically to Prof. Igor Zozoulenko igor.zozoulenko@liu.se and a copy to registrator@itn.liu.se. The deadline is 24 July 2025. **Mark your application in the e-mail subject line with: "postdoc in MIECP, Dnr ITN-2025-00271".** The selection process will start in August due to summer vacation.

Contact:
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