

LINKÖPING UNIVERSITY

# Postdoctoral Scholarship in “Lignin nanoparticles self-assembly and formation through the lens of molecular dynamics simulation”

Laboratory of Organic Electronics, Department of Science and Technology, Linköping University (Campus Norrköping)

## Research environment

At the Laboratory of Organic Electronics (LOE) we explore electronic and optical properties of organic semiconductors, biomaterials from the forest, and hybrid organic materials. We share a common interest in utilizing the combination of electronic and ionic charge for use in healthcare and biology applications, energy, and the internet-of-things. Our research topics include synthesis, material science, theory and modeling, device physics, nanotechnology, biotechnology, and system design. Our activities span the range from basic research to commercialization, the latter carried out in close collaboration with the institute RISE. LOE currently has ~130 researchers and PhD students divided into around 10 research groups, each led by a principal investigator. LOE is also a partner in the Wallenberg Wood Science Center, which is a research center striving for scientific excellence with a focus on new materials from trees. Read more at [www.liu.se/loe](http://www.liu.se/loe)

## Research project

Lignin, the most abundant natural source of aromatic molecules, holds the key to a sustainable future. Despite its prevalence, lignin is one of the most underutilized biopolymers on Earth—primarily burned for energy, wasting its vast potential. This project aims to unlock lignin's transformative capabilities, turning it into a cornerstone for eco-friendly innovations.

Through cutting-edge computational modeling, we will uncover the mechanisms of lignin nanoparticle (LNP) formation, paving the way for groundbreaking applications in drug delivery, nanocomposites, and beyond. Be part of a visionary effort to replace crude oil-derived materials with sustainable, biodegradable alternatives that harness lignin's unique properties.

This project seeks to develop a fundamental understanding of LNP self-assembly through utilizing all atomistic and coarse-grained (CG) molecular dynamics (MD) simulations. For this purpose, novel CG models of lignin will be developed and applied to understand the self-assembly mechanisms of lignin to LNPs. The theoretical studies will be performed in the Theory and Modelling group (<https://liu.se/en/research/laboratory-of-organic-electronics/theory-and-modeling-for-organic-electronics>) under the supervision of Dr. Aleksandar Mehandzhiyski and Prof. Igor Zozoulenko with strong interaction with experimental collaborators from The Royal Academy of Sciences (KTH) and Stockholm University.

### **Qualifications and requirements**

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 computational chemistry, etc.) and needs to be passionate about research.

The applicant must have extensive experience with MD simulations. Experience in coarse-grained modelling is considered a plus. Good skills in programming/scripting are highly desirable. Problem solving ability and creativity, as well as the ability to work independently are essential.

Scholarship may be granted only to non-Swedish citizens with a PhD or equivalent acquired in another country than Sweden. The applicant must not have been employed by Linköping University previously.

### **Starting date**

Spring 2025 or by agreement.

### **Appointment and Conditions**

Appointment is initially for one year with a possibility of an extension for a second year depending on a mutual agreement. The total time for receiving a scholarship from Linköping University can never exceed two years.

The scholarship amounts to SEK28000:-/month (tax-free) (~€2500/month). The scholarship will be received directly from the funder of the project Carl Trygger Foundation.

Travel costs to/from Sweden for a scholarship holder will be covered up to a maximum amount. Funding can be available to participate in conferences.

Essential information about healthcare, insurances etc. can be found [here](#). Questions are welcome to HR@itn.liu.se

### **Application procedure**

The following documents (in pdf-format) must be submitted when applying for a scholarship

- Cover letter, max 1 page, describing your background, research interests and what makes you interested in the position.
- CV, max 2 pages, including contact details to two reference persons.
- Full publication list.
- PhD diploma, and MSc transcripts with grades.

The application should be sent electronically to [aleksandar.mehandzhiyski@liu.se](mailto:aleksandar.mehandzhiyski@liu.se) with cc to [registrator@itn.liu.se](mailto:registrator@itn.liu.se). Mark your application with: MD simulations of lignin **Dnr ITN-2024-00475**, in the e-mail subject field.

Applications deadline: **20 December 2024**.

### **Contact**

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