



UPPSALA
UNIVERSITET

PhD student in AI-aided computational chemistry

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Uppsala University is a comprehensive research-intensive university with a strong international standing. Our ultimate goal is to conduct education and research of the highest quality and relevance to make a long-term difference in society. Our most important assets are all the individuals whose curiosity and dedication make Uppsala University one of Sweden's most exciting workplaces. Uppsala University has over 54,000 students, more than 7,500 employees and a turnover of around SEK 8 billion.

The context of this PhD position is the newly started eSSENCE Graduate school in data-intensive Computing (<https://essenceofscience.se/>). The school is now hiring 10 PhD students at Uppsala University to work on projects that all address the challenge of data-intensive science both from the foundational methodological perspective and from the perspective of data-driven science applications. The present position is one of those ten.

Your host institution will be the Department of Chemistry-Ångström and your affiliated institution will be the Department of Information Technology, both at the Ångström Laboratory of Uppsala University. The Department of Chemistry - Ångström has more than 250 employees and has a turnover of 250 million SEK. [More information is available on our website.](#)

[Read more about our benefits and what it is like to work at Uppsala University](#)

Duties

The main task for a doctoral student is to perform doctoral studies, which includes

both participation in research projects and doctoral courses. The tasks may also include participation in teaching and other departmental work; however, normally to a maximum of 20% of working hours.

The current PhD project concerns machine learning and computer simulations, with the objective to explore atomic-level phenomena. We will build strategies to speed up the way computer simulations are performed and use them to understand the physical/chemical processes that may be important for the functionality of future battery chemistries. Quantum-mechanical calculations, statistical-mechanical simulations, machine learning and data analysis will be tools used in the PhD project.

The supervisors of this PhD position participate in the European research project BIGMAP (<https://www.big-map.eu/>), which stands for "Battery Interface Genome – Materials Acceleration Platform". BIGMAP is one cornerstone in the European Union's objective to reach net-zero CO₂ emissions by year 2050 by means of "Accelerated discovery and design of battery materials, interphases, interfaces and concepts".

Requirements

A competitive candidate should

- have been awarded a second-cycle qualification, or
- have satisfied the requirements for courses comprising at least 240 credits of which at least 60 credits were awarded in the second cycle, or has acquired essentially equivalent knowledge in some other way in Sweden or abroad.
- possess very good oral and written proficiency in English.

We are aware that *not* many students have extensive undergraduate training both in the natural science domain and in the IT domain. In this PhD project we therefore expect the candidate to possess good knowledge in *at least one* of these areas, plus be interested in learning more in the other field (through the research project itself, and also through PhD courses).

Consideration will also be given to good collaborative skills, drive and independence.

Additional qualifications

It is highly desirable that a candidate has studied undergraduate courses in chemistry, physics or engineering equivalent to at least 30 hp.

[Rules governing PhD students are set out in the Higher Education Ordinance chapter 5, §§ 1-7 and in Uppsala University's rules and guidelines.](#)

About the employment

The employment is a temporary position according to the Higher Education Ordinance chapter 5 § 7. Scope of employment 100 %. Starting date 2023-04-01 or as agreed. Placement: Uppsala.

For further information about the position, please contact: Professor Kersti Hermansson (kersti.hermansson@kemi.uu.se; phone 070-4250626) or Dr Peter Broqvist (peter.broqvist@kemi.uu.se), or Dr Per Mattsson (per.mattsson@it.uu.se).

Please submit your application by 27 February 2023, UFV-PA 2023/387.

Are you considering moving to Sweden to work at Uppsala University? [Find out more about what it's like to work and live in Sweden.](#)

Please do not send offers of recruitment or advertising services.

Submit your application through Uppsala University's recruitment system.

Placement: Department of Chemistry - Ångström Laboratory

Type of employment: Full time, Temporary position longer than 6 months

Pay: Fixed salary

Number of positions: 1

Working hours: 100 %

Town: Uppsala

County: Uppsala län

Country: Sweden

Union representative: ST/TCO tco@fackorg.uu.se

Seko Universitetsklubben seko@uadm.uu.se

Saco-rådet sacco@uadm.uu.se

Number of reference: UFV-PA 2023/387

Last application date: 2023-02-27

Apply for position