



Jobbnorge ID: 244157

Deadline: 5/31/2023

Website: <http://www.nmbu.no>

Scope: Fulltime

Duration: Fixed Term

Are you interested in physics-based and data-driven modelling of liquid systems?

PhD position on Machine Learning for Molecular Modelling and Simulation within Data Science

About the position

The Faculty of Science and Technology (REALTEK) at the Norwegian University of Life Sciences (NMBU) invites applications for a full-time doctoral candidate position related to process data technology. The position is for a period of 3 years, or up to 4 years if teaching and other work duties are agreed.

Process data technology is the application of knowledge-driven methods within domains relevant to process engineering - it is one of the fields of research within the Department of Data Science (Institutt for datavitenskap) at REALTEK. The proposed PhD research will evaluate how machine learning based on cellular neural networks can be used to improve molecular models. This doctoral position will be associated with the Department of Data Science, with co-supervision from the Materials Informatics group at REALTEK and external co-supervision by Simula in Oslo (www.simula.no).

A collaboration is foreseen with process/molecular engineering research groups at RPTU Kaiserslautern, TU Berlin, and Imperial College London.

An application for a PhD position at NMBU is at the same time an application for admission to a doctoral programme at the institution. The documentation that is necessary to ensure that the admission requirements are met must be uploaded as an attachment.

Main tasks

The successful candidate is expected to enter a plan for the progress of the work toward a PhD degree during the first months of the appointment, with a view to completing a doctorate within the PhD scholarship period. According to our internal preliminary research plan, subject to further discussion and revision in due course, overall, 36 months' time will be spent on the research activity; thereof, six months are planned for each of the following tasks:

- Familiarization with the methodology and the state of the art.
- Cellular neural network surrogate model of thermodynamic and configurational properties.
- Multicriteria optimization of pair potentials over high-dimensional objective spaces.
- Methodology implementation and assessment for machine learning pair potentials.
- Data integration and force field development for water and aqueous solutions of vanadium.
- Integration and documentation of results, critical discussion, and overarching perspective.

The preliminary research plan (titled "Machine learning for quantitatively reliable and explainable-AI-ready molecular modelling of liquids") is available from martin.thomas.horsch@nmbu.no upon request.

Competence

The successful applicant must meet the conditions defined for admission to a PhD programme at NMBU. The applicant must have an academically relevant education corresponding to a five-year master's degree, with a learning outcome corresponding to the descriptions in the Norwegian Qualification Framework, second cycle. Candidates submitting MSs thesis within 31. May 2023 may be considered. The applicant must have a documented strong academic background from previous studies and be able to document proficiency in both written and oral English. For more detailed information on the admission criteria please see the [PhD Regulations](#) and the relevant [PhD programme description](#).

The applicant must document expertise and interest in the research subject.

Required academic qualifications:

- Master or equivalent diploma or other degree from a course of studies related to process data technology, including but not limited to data science, chemical/mechanical engineering, industrial economics, computer science, chemistry, physics, or applied mathematics.
- Statistical mechanics or thermodynamics competency demonstrated either by a transcript from the course of studies or in another way.
- Programming competency demonstrated either by a transcript from the course of studies or in another way.
- Fulfill all the requirements imposed by law and NMBU's regulations.

Desired competencies (good to have, but can also be acquired on the job):

- Familiarity with common methods/models in molecular simulation.
- Advanced programming competency, including in at least one compiled language such as Fortran, C++, Java, etc., sufficient to co-develop the ms2 code (www.ms-2.de) which is written in Fortran.
- Experience with HPC environments and architectures.
- Some knowledge of semantic technology and/or machine learning.
- If you are interested in a four year contract including teaching, also teaching experience and interest in contributing to teaching within data science.

Industry experience is a plus. If you do not know Norwegian or another Scandinavian language, you will be encouraged and supported at learning Norwegian since it is the main working language at NMBU.

Remuneration and further information

The position is placed in government pay scale position code 1017.

PhD fellows are normally placed in pay grade 54 (NOK 532 200,-) on the Norwegian Government salary scale upon employment and follow ordinary meriting regulations.

Employment is conducted according to national guidelines for University and Technical College PhD scholars.

The engagement is to be made in accordance with the regulations in force concerning State Employees and Civil Servants, and the acts relating to Control of the Export of Strategic Goods, Services and Technology.

Candidates who by assessment of the application and attachment are seen to conflict with the criteria in the latter law will regrettably be prohibited from recruitment to NMBU.

For further information, you can contact Dr Martin Thomas Horsch, e-mail: martin.thomas.horsch@nmbu.no.

[Information for PhD applicants](#) and [general Information to applicants](#)

Application

To apply online for this vacancy, please click on the 'Apply for this job' button above. This will route you to the University's Web Recruitment System, where you will need to register an account (if you have not already) and log in before completing the online application form. Applicants invited for an interview are expected to present original diplomas and certificates.

Application deadline 31st May 2023.

The following documents must be attached to the application:

- Cover letter (maximum 1 page).
- CV, including a list of scientific publications if you have any. Do not attach any publications in PDF format, providing links is sufficient.
- Certified copies of the relevant academic diplomas and certificates. Diplomas, transcripts, and diploma supplements that are not in English or Norwegian (or a language very close to Norwegian) must be uploaded both in the original version and as an English translation. Graduates of universities outside Norway are requested to enclose a diploma supplement or a similar document, describing the study programme and the grading system at a sufficient level of detail.
- Documentation of proficiency in written and oral English in accordance with [NMBU PhD regulation section 5-2 \(3\)](#).
- Names and contact details for two references.
- Any additional relevant documentation of professional knowledge.
- Confirmation that information and documentation submitted via the job application can be used for the admissions process at NMBU.

About The Faculty of Science and Technology

[The Faculty of Science and Technology \(REALTEK\)](#) develops research-based knowledge and educates civil engineers and lecturers needed to reach the UN's sustainability goals. We have approximately 150 employees, 70 PhD students and soon 1500 students. The education and research at REALTEK cover a broad spectrum of disciplines.

This includes data science, mechanics and process engineering, robotics, construction and architecture, industrial economics, environmental physics and renewable energy, geomatics, water and environmental engineering, applied mathematics as well as secondary school teacher education in natural sciences and use of natural resources such as in agriculture, forestry and aquaculture. The workplace is in Ås, 30 km from Oslo.

What is it really like to work at the Faculty of Science and Technology (REALTEK) at NMBU?

- [Guided tour of the Faculty of Science and Technology on Vimeo](#)

The Norwegian University of Life Sciences (NMBU)

NMBU's focus is a joint effort for a sustainable future. Our university will contribute to securing the future of life, through outstanding research, education, communication and innovation.

NMBU has 1,900 employees of which about 500 phd scholarships and 6,700 students. The university is divided into seven faculties.

NMBU believes that a good working environment is characterised by diversity.

We encourage qualified candidates to apply regardless of gender, functional ability, cultural background or whether you have been outside the labour market for a period. If necessary, workplace adaptations will be made for persons with disabilities. More information about NMBU is

available at www.nmbu.no.

Additional information

Place of service:

Universitetstunet 3 1430 Ås (Ås Municipality)