



UNIVERSITETET  
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**Jobbnorge ID:** 263373

**Deadline:** 6/13/2024

**Website:** <http://www.uio.no/>

**Scope:** Fulltime

**Duration:** Engagement

## Researcher in Computational Chemistry

### About the position

Position as Researcher is available at the [Hylleraas Centre for Quantum Molecular Sciences](#), Department of Chemistry.

The position is for a period for up to 2.5 years.

Starting date is no later than 01.08.2024.

### Knowledge development in a changing world - Science and technology towards 2030

The Faculty of Mathematics and Natural Sciences

Video: <https://www.youtube.com/watch?v=t4wvWQEHdEs>

### Job description/project description:

Applicants are invited to apply for a 2.5-year position as a researcher in computational chemistry on the Research Council of Norway Young research talent project **Harnessing Hydrogen** by **Optimized Ion-Conductive Metal-Organic Frameworks (H<sub>2</sub>O-MOF)** to be based at the Department of Chemistry, University of Oslo.

The development of fuel cell technology capable of efficiently converting hydrogen into electricity is considered a critical component in the transition away from CO<sub>2</sub>-emitting energy sources. In this regard, ion exchange membrane fuel cells are gathering considerable interest due to their high electricity conversion rates. However, this technology's full commercial potential is held back by the performance-critical ion exchange membranes (IEM) failing to meet the challenges of achieving high ion conductivity, low manufacturing cost, and high robustness. Porous metal-organic frameworks (MOFs) exhibit channels that facilitate ion conduction, high structural stability, and chemical tunability, making MOFs a promising material for the next generation of IEMs. To exploit the full potential of MOFs, i.e., to rationally design MOFs, there is a need for knowledge of the underlying molecular mechanisms behind ion conduction inside MOFs.

The overall goal of the research project is:

- To develop and apply machine learning potentials (MLP) to model, understand, and optimize proton and hydroxide conductivity of metal-organic frameworks for potential use as ion exchange membranes in fuel cells.

This will be achieved by:

- Developing and expanding in-house active learning software for efficient and robust parametrization of MLPs and developing automated pipelines for the determination of proton- and hydroxide conductivity in MOFs.

This work will be conducted in collaboration with experimental collaborators at the catalysis section University of Oslo, and modeling experts at the University of Ghent. The researcher will be hosted at the Hylleraas Centre for Quantum Molecular Sciences, a national center of excellence.

### Qualification requirements:

The Faculty of Mathematics and Natural Sciences has a strategic ambition to be among Europe's leading communities for research, education and innovation. Candidates for these fellowships will be selected in accordance with this, and expected to be in the upper segment of their class with respect to academic credentials.

- Applicants must hold a degree equivalent to a Norwegian doctoral degree in chemistry, physics, applied mathematics, informatics, computer science, or related fields. Doctoral dissertation must be submitted for evaluation by the closing date. Only applicants with an approved doctoral thesis and completed defence are eligible for appointment
- Fluent oral and written communication skills in English

Demonstrated experience in the following fields is required by the applicants:

- Molecular dynamics
- Software development
- Git
- Machine learning

- HPC
- Statistical mechanics/thermodynamics

### Personal skills:

- Excellent teamwork capabilities, social skills
- Ability to work independently and take initiative

### We offer:

- Salary NOK minimum 575 400 - 696 611 per annum depending on qualifications in position as Researcher (position code 1109)
- Attractive [welfare benefits](#) and a generous pension agreement
- Professionally stimulating working environment
- Vibrant international academic environment
- Oslo's family-friendly surroundings with their rich opportunities for culture and outdoor activities

### The application must include:

- Cover letter (statement of motivation, summarizing scientific work and research interest)
- CV (summarizing education, positions, pedagogical experience, administrative experience and other qualifying activity)
- Copies of educational certificates, academic transcript of records **and letters of recommendation**
- A complete list of publications and up to 5 academic works that the applicant wishes to be considered by the evaluation committee
- Names and contact details of 2-3 references (name, relation to candidate, e-mail and telephone number)

The application with attachments must be delivered in our electronic recruiting system, please follow the link "apply for this job". Foreign applicants are advised to attach an explanation of their University's grading system. Please note that **all** documents should be in English (or a Scandinavian language).

In assessing the applications, special emphasis will be placed on the documented, academic qualifications, as well as the candidates motivation and personal suitability. Interviews with the best qualified candidates will be arranged.

It is expected that the successful candidate will be able to complete the project in the course of the period of employment.

### Formal regulations:

According to the Norwegian Freedom and Information Act (Offentleglova) information about the applicant may be included in the public applicant list, also in cases where the applicant has requested non-disclosure.

The University of Oslo has an [agreement for all employees](#), aiming to secure rights to research results a.o.

The University of Oslo aims to achieve a balanced gender composition in the workforce and to recruit people with ethnic minority backgrounds.

### Contact persons:

For further information about the position, please contact:

Researcher Sigbjørn Løland Bore, phone number: +47 928 81 237, e-mail: [s.l.bore@kjemi.uio.no](mailto:s.l.bore@kjemi.uio.no)

Head of Office Jan Ingar Johnsen , phone number: +47 228 54 826, e-mail: [j.i.johnsen@kjemi.uio.no](mailto:j.i.johnsen@kjemi.uio.no)

For technical questions regarding the recruitment system, please contact:

HR-adviser Olga Holmlund, e-mail: [olga.holmlund@mn.uio.no](mailto:olga.holmlund@mn.uio.no).

## About the University of Oslo

**The University of Oslo** is Norway's oldest and highest rated institution of research and education with 28 000 students and 7000 employees. Its broad range of academic disciplines and internationally esteemed research communities make UiO an important contributor to society.

**Hylleraas Centre for Quantum Molecular Sciences** operates under the aegis of the Department of Chemistry at the Faculty of Mathematics and Natural Sciences. The Department of Chemistry is Norway's largest institution within research and education in chemistry. Our research excels internationally and we educate students to a wide variety of jobs in industry, academia, research institutions, schools and public administration.

Our research ranges from the core topics of chemistry to applied science within in environmental, health, energy and materials. The Department has extensive contacts with industry, research and educational institutions at home and abroad.

As partner in the Centre for Materials Science and Nanotechnology our researchers contributes to a significant interdisciplinary efforts in cooperation with the Department of Physics. The Department of Chemistry has its own school laboratory as a great resource for teachers, public outreach and the didactics of chemistry.

### Additional information

**Place of service:**

Problemveien 7 0313 Oslo (Oslo Municipality)