

Jobbnorge ID: 280277 Deadline: 6/2/2025

Website: http://www.uio.no/

Scope: Fulltime

Duration: Temporary

# Researcher position in chemistry related to computations-based design for C-H activation reactions

# About the position

A position as a Researcher in chemistry is available at the Centre for Materials Science and Nanotechnology (SMN), University of Oslo.

The position is for a period of 1 year, with possible extension, upwards limited to the project end date (31.10.2026).

The starting date is no later than November 1, 2025.

### More about the position / Job description

The position is associated with an EU funded ERC-Synergy Grant (ERC-SyG) project <u>Unravelling the secrets of Cu-based catalysts for C-H activation (CUBE) (cube-synergy.eu)</u>. The aim of the CUBE project is to understand the key mechanistic features of copper-catalyzed C-H activation via a holistic approach in which biological and synthetic catalysts are studied side by side. The ultimate goal is the selective production of methanol from CH4 and O2. A promising strategy is to incorporate bioinspired catalytic motifs and second sphere components in solid porous materials, combining heterogeneous and homogeneous catalytic approaches. The unprecedented tunability, stability and high surface area of metal-organic frameworks (MOFs) make them attractive as solid framework for this purpose.

Metal complex and materials synthesis, characterization, performance testing and mechanistic studies - using experimental and computational tools - are performed in a direct feed-back loop, involving organic and inorganic synthesis chemists, spectroscopists, computational chemists and enzymologists. The resulting design principles will be used to develop new catalysts with rationally designed functionality.

CUBE is a joint project between the University of Oslo (Norway), the Norwegian University of Life Sciences (Norway), the University of Turin (Italy) and the Max-Planck Institute for Chemical Energy Conversion (Germany).

The ERC-SyG project scheme implies that the successful candidates will collaborate closely with colleagues at all partner institutions, by regular virtual and physical meetings, by sample and data exchange, and by shorter and longer research stays at partner institutions.

The Researcher will work with other researchers to apply computational methods to study C-H bond activation reactions catalysed by Cu-based single-site metal-organic frameworks. Special attention will be paid to second coordination sphere interactions established between the linkers, the oxidant, and the substrate. A machine learning approach will be used to screen MOF databases and newly synthesized linkers.

The Researcher will work in a highly international and interdisciplinary team collaborating closely with experimental chemists. Access to state-of-the-art supercomputing facilities will be given.

The position will be part of the Section for catalysis and organic chemistry. The <u>Section for catalysis and organic chemistry</u> studies the correlation between catalyst composition/structure and their effects on chemical reactions. The catalysts can be of organic and/or inorganic origin. The section has approximately 35 members, subdivided into three groups: the zeolite group synthesizes and characterizes zeolite and zeotype materials and studies catalytic reactions over those materials; the MOF-group does the same with metal-organic frameworks; the homogenous catalysis group synthesizes metal-organic complexes and studies their catalytic reactions.

The Section for catalysis and organic chemistry is part of Centre for Materials Science and Nanotechnology (SMN). Centre for Materials Science and Nanotechnology is an interdisciplinary centre, collaboration between five research groups in physics and chemistry, and spearheads the MN Faculty's efforts for sustainable energy solutions. The Centre comprises UiO's focus on renewable energy, materials science, and nanotechnology.

The Section for catalysis and organic chemistry has strong ties to the Hylleraas Centre for Quantum Molecular Science.

Employment in the Section for catalysis and organic chemistry will enable the successful candidate to work in a highly cross-disciplinary field in an internationally competitive research group.

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

#### **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 fellowships will be selected in accordance with this and are 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 or a related field. Doctoral dissertation must be submitted for evaluation by the closing date. Only applicants with an approved doctoral thesis and public defence are eligible for appointment.
- Documented experience using DFT methods for studying reaction mechanisms with metal organic complexes.
- Previous experience in grand canonical Monte Carlo (GCMC) simulations.
- Programming skills and previous experience in Machine Learning (ML).
- Fluent oral and written communication skills in English.
- The position's subject area may require licensing under the Norwegian Export Control Act. In order to be considered for the position, it is
  a prerequisite that UiO must be able to be granted such license: <a href="https://www-int.uio.no/english/for-employees/support/international-cooperation/responsibility/export-control/index.html">https://www-int.uio.no/english/for-employees/support/international-cooperation/responsibility/export-control/index.html</a>

#### **Desired qualifications:**

- · Previous experience in the use of QM/MM for reactivity studies and MOF da-ta handling
- Knowledge of C-H bond activation reactions
- · Experience working on collaborative projects with experimental researchers

# Personal skills

- Ability to conduct high-quality independent research within a broad collaboration
- · Strong communication skills and the ability to work as part of a team
- · Willingness to work together with PhD and/or Master/Bachelor students in speciality field
- · Self-motivation, creativity, genuine curiosity about the subject, work discipline, professional ethics, and ambition

# We offer / We can offer you / Why should you choose us?

- Exciting and meaningful tasks in an organization with an important societal mission, contributing to knowledge development, education, and enlightenment that promote sustainable, fair, and knowledge-based societal development.
- · Committed colleagues in a good working environment. A pleasant and stimulating work environment
- Good welfare schemes.
- Opportunity of up to 1.5 hours a week of exercise during working hours.
- A workplace with good development and career opportunities.
- Membership in the <u>Statens Pensjonskasse</u>, which is one of Norway's best pension schemes with beneficial mortgages and good insurance schemes.
- Salary in position as Researcher, position code 1109 in salary range NOK from 579 700 to 708 000 per annum, depending on competence and experience. From the salary, 2 percent is deducted in statutory contributions to the State Pension Fund.

Read more about the benefits of working in the public sector at Employer Portal.

### Inclusive worklife and diversity at UiO

Inclusion and diversity are a strength. The University of Oslo has a personnel policy objective of achieving a balanced gender composition. Furthermore, we want employees with diverse professional expertise, life experience and perspectives.

If there are qualified applicants with disabilities, employment gaps or immigrant background, we will invite at least one applicant from each of these categories to an interview.

We hope that you will apply for the position.

### **Application**

Your application should include:

- Cover letter (statement of motivation, summarizing scientific work and research interest, and how this relates to the targeted position)
- CV (summarizing education, positions, pedagogical experience, administrative experience and other qualifying activity)
- · Copies of educational certificates and academic transcript of records
- 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)

Application with attachments must be submitted via our recruitment system Jobbnorge, click "Apply for the position".

When applying for the position, we ask you to retrieve your education results from <u>Vitnemålsportalen.no</u>. If your education results are not available through Vitnemålsportalen, we ask you to upload copies of your transcripts or grades. Please note that all documentation must 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 applicant's motivation and personal suitability.

#### **General information**

The best qualified candidates will invited for interviews.

Applicant lists can be published in accordance with Norwegian Freedom of Information Act § 25. When you apply for a position with us, your name will appear on the public applicant list. It is possible to request to be excluded from this list. You must justify why you want an exemption from publication and we will then decide whether we can grant your request. If we can't, you will hear from us.

Please refer to Regulations for the Act on universities and colleges chapter 3 (Norwegian) and Rules for the use of research posts SKO 1108, 1109, 1110 and 1183 at UiO.

The University of Oslo has a transfer agreement with all employees that is intended to secure the rights to all research results etc.

# **University of Oslo**

**The University of Oslo** is Norway's oldest and highest rated institution of research and education with 26 500 students and 7 200 employees. Its broad range of academic disciplines and internationally esteemed research communities make UiO an important contributor to society.

Centre for Materials Science and Nanotechnology (SMN) is an interdisciplinary focus field for material and energy research at the University of Oslo. SMN has focused on basic research in renewable energy and environmentally friendly use of fossil energy sources.

The center consists of research groups from the Department of Physics and the Department of Chemistry, has about 100 employees from around the world and manages more than 80 projects funded by EU, RCN and others.

### Additional information

#### **Contact persons:**

- For further information please contact Ainara Nova, Researcher Phone: +4746221700 | E-mail: Ainara.nova@kjemi.uio.no
- For questions regarding Jobbnorge, please contact Elin Thoresen, HR Adviser Phone: | E-mail: elithore@mn.uio.no

#### Place of service:

Problemveien 7 0313 Oslo (Oslo Municipality)