Jobbnorge ID: 280173
Deadline: 6/15/2025
Website: http://www.ntnu.no
Scope: Fulltime
Duration: Temporary

The Department of Physics has a vacancy for a

PhD Candidate in computational material research at the Materials Theory Group

This is NTNU

NTNU is a broad-based university with a technical-scientific profile and a focus in professional education. The university is located in three cities with headquarters in Trondheim.

At NTNU, 9,000 employees and 43,000 students work to create knowledge for a better world.

You will find more information about working at NTNU and the application process here.

Video: https://youtu.be/Xt-yHCN5QS0

About the position

We have a vacancy for a PhD position in the Materials Theory group at the Department of Physics, Norwegian University of Science and Technology (NTNU) in Trondheim, Norway. We are looking for a skilled and ambitious candidate to join the **DYNCAT** project, funded by the Research Council of Norway (NFR).

DYNCAT aims to develop highly predictive, physics-based models to study and optimize the Rochow Mülller process, which generates the raw material for silicone production. The project will focus on improving production efficiency and control through the use of particle-based simulation techniques to investigate the catalytic mechanisms and the formation of dichlorodimethylsilane (M2), the key product of the Rochow-Müller reaction.

The successful candidate will work in an international research environment and contribute to the computational modelling efforts at the Materials Theory Group. We are seeking a candidate with a strong theoretical background in **condensed/soft matter physics** or **physical chemistry**, a keen interest in **programming**, and strong motivation to develop new computational models for natural physical processes with real-world industrial applications. The candidate will also collaborate actively with research scientists at **SINTEF Industry**, who have expertise in **experimental and theoretical catalysis**, **surface science**, and **adsorption processes**. This PhD position is for a period of **three years**. The goal is to complete a doctoral education leading to the award of a PhD degree. The position will be supervised by **Associate Professor Raffaela Cabriolu** (Department of Physics, NTNU) as the main supervisor and **Dr. Francesca L. Bleken** (Senior Scientist, SINTEF Industry) as co-supervisor.

Your immediate leader will be the Head of Department.

Duties of the position

- Develop and test new models and protocols using classical simulation methods such as **Molecular Dynamics (MD)** and **Monte Carlo (MC)**, as well as quantum approaches like **Density Functional Theory (DFT)**.
- Develop novel **Graph Neural Network (GNN) potentials** to accurately represent the catalytic behavior of specific species involved in silicone formation.
- Benchmark classical simulation results against **DFT simulations** and **validate all modelling predictions** through comparison with available literature data.
- Perform **high-performance computing (HPC)** simulations to analyze and visualize time-dependent molecular properties.
- Collaborate with an interdisciplinary team of researchers and actively participate in discussions and knowledge exchange within the project.
- Present research findings at international conferences and publish scientific results in **peer-reviewed journals**.
- Participate in the research group Materials Theory Group.

Be prepared for changes to your work duties after employment.

Required selection criteria

- You must have an academically relevant background within computational physics.
- You must have a Master's degree in computational physics. Your course of study must correspond to a five-year Norwegian course, where 120 credits have been obtained at master's level.
- You must have a strong academic background from your previous studies and have an average grade from your Master's degree study, or equivalent education, which is equal to B or better compared to NTNU's grading scale. If you do not have letter grades from previous studies, you must have an equally good academic foundation. If you have a weaker grade background, you may be considered if you can document that you are particularly suitable for a PhD education.
- You must meet the requirements for admission to the Doctoral Programme in Physics.
- The position requires spoken and written fluency in the English language

PLEASE NOTE: For detailed information about what the application must contain, see paragraph "About the application".

The appointment is to be made in accordance with Regulations for the Universities and Colleges Act (university and colleges regulations) and Regulations for the degrees philosophiae doctor (ph.d.) and philosophiae doctor (ph.d.) in artistic development work at the Norwegian University of Science and Technology (NTNU) for general criteria for the position.

Preferred selection criteria

- A documented background in computational physics is required with a focus on atomistic modelling (Molecular Dynamics, Monte Carlo and/or density Functional Theory)
- The applicant must have good programming skills in at least one of the following programming languages: C/C++ and/or Python, Julia is a plus.
- Prior experience in **molecular simulations**, **machine learning techniques**, and **programming** is highly desirable.
- Genuine interest in deep graph neural networks models.

Personal characteristics

To complete a doctoral degree (PhD), it is important that you are able to:

- Work independently
- Work in a structured way, set goals and make plans to achieve them
- Present and discuss your research with other professionals
- Get involved and contribute constructively with feedback
- Work constructively under pressure or in the face of adversity
- Show curiosity and a strong motivation for the subject
- Analyze data, assess different perspectives and draw well-founded conclusions
- Be flexible and open to adjusting the plan for the project as needed
- Other characteristics
- Other characteristics

Emphasis will be placed on personal qualities.

We offer

- An exciting job with an important mission in society
- Developing tasks in a strong and international professional environment
- Career guidance and follow-up during the PhD period
- Open and inclusive working environment with committed colleagues
- Working capital that can be used to implement the project
- Mentor programme as a new employee at NTNU
- As a public employee, you have favourable benefits as a member of the Norwegian Public Service Pension Fund (SPK)

You will be employed as a PhD Candidate at NTNU and will have access to employee benefits and discounts.

Diversity

Diversity is a strength, and at NTNU we aim to be an employer that reflects the diversity in society and that makes use of the potential of the population's collective skills. Our vision is Knowledge for a better world and our values are creative, critical, constructive and respectful. We believe that an organization that is equal, diverse and gender-balanced is essential for us to achieve our goals.

We strive to attract employees with different skills, life experiences and perspectives to contribute to even better problem solving of our societal mission in research and education.

If you think this position is relevant and interesting, we encourage you to apply, regardless of gender, functional ability and cultural background, or whether you have been out of work for a period of time.

At NTNU we want to increase the proportion of women in scientific positions. We have a number of measures to promote equality. (delete if not applicable)

Salary and conditions

In the position of PhD Candidate, code 1017, your gross salary will normally be NOK 536 200,- per annum. A 2% statutory contribution to the State Pension Fund is deducted from the salary.

The employment period is 3 years.

For employment as a PhD Candidate, it is a prerequisite that you gain admission to the PhD programme in physics within three months of your employment contract start date, and that you participate in an organized doctoral programme throughout the period of employment.

As an employee at NTNU, it is important that you keep yourself up to date with academic and organizational changes and adapt to them.

For the necessary academic and social interaction, it is a prerequisite that you are physically present and available to the institution on a daily basis.

The appointment is carried out in accordance with the principles of the State Employees Act, and Export control(legislation that regulates the export of knowledge, technology and services). Candidates who, after assessment of the application and attachments, are considered to be in conflict with the criteria in the latter act, will not be able to be employed.

About the application

The attachments must accompany the application as these documents form the basis of the application assessment. The documents must be in English.

Please note: the application will only be assessed on the basis of the information we have received by the application deadline. Therefore, make sure that your application clearly shows how your skills and experience meet the criteria described above. The application and all attachments must be sent electronically via Jobbnorge.no. If you are invited to an interview, you must bring certified copies of certificates The application must include:

- Transcripts and diplomas for Bachelor's and Master's degrees
- CV
- Copy of Master's thesis. If you have recently submitted your Master's thesis, you can attach a draft of the thesis. Documentation of a completed Master's degree must be presented before taking up the position.
- Short letter of motivation (400 words/1 page)
- Names and contact information of three relevant referees

If all, or parts, of your education has been taken abroad, we also ask you to attach documentation of the scope and quality of your entire education, both Bachelor's and Master's education, in addition to other higher education. If your institution uses “diploma supplement” (normal for most European institutions), you must attach this. A description of the documentation required can also be found here. If you already have a statement from Norwegian Directorate for Higher Education and Skills (HK-dir), please attach this as well.

Joint works will be considered. If it is difficult to identify your contribution to joint work, you must attach a brief description of your participation.

When assessing the best qualified, we emphasize necessary qualifications such as education, experience and personal suitability. Motivation for the position, ambitions and potential for research will also count when assessing the candidates.

NTNU recognizes a wide range of academic contributions and has committed itself to The San Francisco Declaration on Research Assessment and CoARA (responsible assessment of research and recognition of a greater breadth of academic contributions in accordance with NTNU's social mission).

General information

A public list of applicants with name, age, job title and municipality of residence is prepared after the application deadline. If you wish to be exempt from entry on the public applicant list, this must be justified. Assessment will be made in accordance with current legislation. You will be notified if the exemption is not granted.

If you think this position looks interesting and in line with your qualifications, you are welcome to apply.

If you have any questions about the position, please contact Associate Professor Raffaela Cabriolu ,email raffaela.cabriolu@ntnu.no.

If you have any questions about the recruitment process, please contact HR advisor Magnus Gautvik, e-mail: magnus.gautvik@ntnu.no.

Application deadline: 15.06.2025

For practical information about working at NTNU, please visit this webpage.

The city of Trondheim is a modern European city with a rich cultural scene. Trondheim is the tech capital of Norway with a population of 200,000. The Norwegian welfare state, including healthcare, schools, kindergartens and overall equality, is probably the best of its kind in the world. Professional subsidized day-care for children is easily available. Furthermore, Trondheim offers great opportunities for education (including international schools) and possibilities to enjoy nature, culture and family life and has low crime rates and clean air quality.

NTNU - knowledge for a better world

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The Norwegian University of Science and Technology (NTNU) creates knowledge for a better world and solutions that can change everyday life.

Department of Physics

Our research and teaching are both experimental and theoretical, covering a wide range of disciplines. Our activities contribute to development of new medical technology and to finding solutions for the next generation’s communication technology, energy utilization and development of materials. The Department of Physics is one of eight departments in the Faculty of Natural Sciences.

Additional information

Place of service:

Høgskoleringen 1 7491 Trondheim (Trondheim Municipality)