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Nettside: <http://www.ntnu.no>
Omfang: Heltid
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The Department of Materials Science and Engineering has a vacancy for a

PhD Candidate in Quantum Simulations of Solid-State Li-ion Battery Materials

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

A PhD candidate position in the field of atomic simulations for the development of solid-state Li-ion batteries is available. For the position as a PhD candidate, the goal is a completed education up to an obtained doctoral degree.

The academic position will provide the opportunity for professional development through studies towards a PhD degree, related to the TEASE project (Tuneable and Earth Abundant Solid-State Li-ion Batteries). The TEASE project aims to engineer new tuneable materials for Earth-abundant solid-state electrolytes using atomistic simulations (primarily density functional theory, DFT, and molecular dynamics, MD) as well as developing machine learning models to accelerate this.

The tasks for the PhD candidate will cover the development of new solid-state electrolytes. The position involves a mixture of first principles materials simulations (density functional theory, ab-initio molecular dynamics), machine learning, and python coding, with the use of national supercomputing architecture. Within these simulations, the candidate will perform calculations regarding thermodynamic stability, phonons, defects and doping, ionic conductivity, as well as develop analysis tools and methods for the scientific community.

The successful candidate will be affiliated to the FACET research group at the Department of Materials Science and Engineering at NTNU and work in a multidisciplinary and international environment. Information about the research group can be found [here](#).

The main supervisor for this project will be Dr Benjamin A. D. Williamson, and will work in collaboration with the group of Professor Daniel Rettenwander for experimental realisation of promising results.

The main workplace will be Trondheim.

Duties of the position

The PhD candidate will be involved in the discovery and development of new stable solid-state electrolytes with high ionic conductivity. This will involve performing calculations using density functional theory (DFT) to simulate thermodynamic stability of novel compounds, band alignment, phonons, defects and doping, solid solutions and disorder, as well as ionic conductivity for a holistic overview. In addition, ab-initio molecular dynamics (with machine learned forcefields) will be employed for both ionic conductivity, and phase transitions. Within this position, national supercomputing architecture [SIGMA2](#) will be used, as well as python coding for analysis. The PhD student will plan and conduct calculations according to the project objectives with support from the supervisor. The results of the project are expected to be published in scientific journals and presented at national and international conferences.

Required selection criteria

- You must have a professionally relevant background in materials chemistry, materials science and engineering, nanotechnology or materials and solid-state physics.
- Familiarity with basics of Li-ion battery materials, and/or functional materials in general.
- Your education must correspond to a five-year Norwegian degree program in Materials Science and Engineering or equivalent, where 120 credits are obtained at master's level.

- You must have a strong academic background from your previous studies and an average grade from the master's degree program, or equivalent education, which is equal to B or better compared with NTNU's grading scale. If you do not have letter grades from previous studies, you must have an equally good academic basis. If you have a weaker grade background, you may be assessed if you can document that you are particularly suitable for a PhD education.
 - Master's students who expect to complete their studies by summer 2025 are encouraged to apply. Master's degree must be completed before starting the position.
 - You must meet the requirements for admission to the [Faculty of Natural Sciences doctoral program](https://www.ntnu.edu/nv/phd) <https://www.ntnu.edu/nv/phd>
 - You must be able to communicate fluently in English and have good communication skills.

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 strong background and hands-on experience in functional materials, e.g. battery materials is desired.
- Knowledge of inorganic chemistry is an advantage.
- Python (or related) coding/troubleshooting or experience with the UNIX environment is an advantage.
- Knowledge of a Scandinavian language is considered as a plus.

Personal characteristics

In the evaluation of which candidate is best qualified for the PhD position, emphasis will be placed on education, experience, and personal suitability. The candidate should:

- Be creative and innovative
- Take responsibility for their own progress and be able to work independently
- Be able to collaborate closely with other members of the FACET research team
- Be diligent and able to show initiative on behalf of own work
- Be structured, targeted, and solution-oriented
- Have good interpersonal skills that allow for a positive and friendly attitude and contribute to a sustainable social environment

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.

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. If learning Norwegian (level A2 corresponding to at least 15 credits) is to be completed before the end of the employment period, the employment period can be extended by 10 weeks after completed and documented the Norwegian course.

For employment as a PhD Candidate, it is a prerequisite that you gain admission to the [PhD programme in Materials Science and engineering](https://www.ntnu.edu/studies/phmt) (<https://www.ntnu.edu/studies/phmt>) 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 (including a description of your scientific work) must accompany the application as these documents form the basis of the application assessment. The documents must be in Norwegian or 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 upon request.

The application must include:

- A cover letter describing the personal motivation, summarising scientific work, and how the applicant sees their background suitable
- A draft research proposal (2 pages) for the PhD study, presenting ideas for the PhD-work and how it can be applied, based on the project description given in this advertisement. This proposal will be neither final nor binding for the project
- CV, certificates and diplomas
- Transcripts and diplomas for bachelor's and master's degrees. If you have not completed the master's degree, you must submit a confirmation that the master's thesis has been submitted.
- Name, address and contact information of three referees
- Documentation of English language proficiency (if applicable)
- Publications or other relevant research work if available

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 Dr Benjamin A. D. Williamson, email: benjamin.williamson@ntnu.no.

If you have any questions about the recruitment process, please contact HR-consultant Marie Kristiansen, email: marie.kristiansen@ntnu.no.

Application deadline: 25.05.2025

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 Materials Science and Engineering

We are Norway's leading educational and research environment in materials engineering, materials chemistry and materials science. In collaboration with business and industry, we are a driving force for the development of innovative materials as well as new applications and manufacturing processes. Activities in our disciplines are vital for the green shift. [The Department of Materials Science and Engineering](#) is one of eight departments in the [Faculty of Natural Sciences](#).

Tilleggsinformasjon

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