

 Targeted job

## DTU Global Top Student Programme - Internship in Machine Learning for Atomistic Simulations



**DTU Energy**

Government/ Charity/ Public Institution/ Other  
Engineering

Published on 23 June 2026

Contract

**Internship 4 to 9 months**

Location

**Kongens Lyngby, Region Hovedstaden (Denmark)**

Start date

**January 2027**


Salary

**Information not provided**

Remote working

**No remote working**

The Technical University of Denmark (DTU) is one of Europe's leading engineering universities, known for excellence in research, education, innovation, and scientific advice. We work closely with industry and international partners to apply science and technology for societal benefit in an interdisciplinary and inclusive environment.

This internship is offered through DTU's Global Top Student Programme. Only top bachelor students nominated by their home university are eligible to apply. As participants, you will join a  our academic environment where theory meets practice, and students develop both professionally and personally.

## Job Description

DTU Energy is part of DTU and focuses on the research and development of functional materials, components, and systems for sustainable energy conversion and storage technologies, with the mission of supporting the green transition by enabling efficient generation, conversion, and storage of energy from renewable sources.

The department works at the forefront of fuel cells and electrolysis, batteries, power-to-X and green fuels, solar energy harvesting, and the design of advanced materials for clean-energy applications, combining research, education, and collaboration with external partners. The department is characterized by a collaborative culture, high academic standards, and a strong focus on innovation and real-world impact.

You will join the Autonomous Materials Discovery section within the department. The team consists of researchers, postdocs, PhD students, development engineers, and scientific software developers working closely together on developing methods, tools, and hardware, including machine learning, digital twins, FAIR data workflows, and autonomous laboratories, that accelerate the pace of materials discovery for energy applications, often in close collaboration with the CAPeX Pioneer Center for Accelerated Materials Discovery. As an intern, you will work closely with experienced colleagues who will support your learning and development, while also giving you the opportunity to contribute your own ideas and skills.

This project in particular focuses on the interface between machine learning and atomistic simulations, with an emphasis on developing models that can accelerate the study of complex molecular systems such as enzymes relevant to sustainable energy conversion. You will explore how modern ML approaches can be combined with established atomistic simulation techniques to bypass bottlenecks that currently limit the throughput and accuracy of computational screening. Depending on your interests and prior experience, the project can be tailored toward methodological development (e.g., new architectures, training schemes, or sampling algorithms), application-driven studies of specific systems, or a combination of both. We are particularly interested in candidates with a background in machine learning who are curious about chemistry and physics-informed modeling; familiarity with atomistic simulations is welcome but not required, as you will be supported by colleagues with deep expertise in the field.

Your tasks will include (but are not limited to):

- Supporting ongoing research or development projects
- Collecting, processing, and analyzing data
- Assisting with simulations and technical analyses
- Contributing to reports, presentations, or scientific documentation
- Participating in team meetings and project discussions

- Collaborating with internal and external stakeholders

The exact tasks and responsibilities will be adjusted based on your background, interests, and the needs of the team.

### **Approval and qualifications**

We are looking for a motivated and curious candidate who:

- Is currently enrolled in the final year of a Bachelor's degree programme
- Has a background in either Machine Learning, Chemistry, Biochemistry, or Physics
- Has relevant academic or practical experience (coursework, projects, student jobs, etc.)
- Has an interest in machine learning methods applied for atomistic systems
- Is analytical, structured, and able to work independently
- Has good collaboration and communication skills
- Has demonstrated proficiency in written and spoken English, documented by one of the following English language tests. Minimum required scores are:
  - Duolingo English Test (overall: 120)
  - TOEFL (old scale overall: 92, new scale overall: 4.5)
  - IELTS Academic (overall: 6.5)
  - CAE (overall: 180)

You can read more about the language test requirements [here](#).

### **What we offer**

DTU offers a prestigious internship at the Lyngby Campus in Greater Copenhagen, providing hands-on research experience in an international academic environment. Interns collaborate with leading researchers on advanced projects while developing their professional skills in a supportive setting.

Living in Greater Copenhagen also offers international students a high quality of life, a strong academic community, and a vibrant city experience in Denmark's capital region.

As part of the internship, the student will also become a member of DTU's alumni community network, gaining access to a range of exclusive offers and support, including:

- Administrative and practical support – assistance with residence permits, housing, etc.
- Social and networking framework, including an introduction week, cultural activities, and semester events
- Parallel academic opportunities – coursework on the side

## **Practical information:**

- Internship period: 25 January 2027 – 25 June 2027 (one semester) or until 18 December 2027 (two semesters)
- Working hours: 25–37 hours per week, either full-time or part-time depending on whether the student chooses to take courses alongside the internship.
- Location: DTU Lyngby Campus in the Greater Copenhagen area
- Compensation: This is an unpaid internship

You can read more about the department here: <https://www.energy.dtu.dk/>

For useful information on the programme and student life at DTU, see [Global Top Student Programme](#) and [Student guide - DTU](#).

## **Application procedure**

The application procedure consists of two steps.

### **Step 1: Nomination**

In order to be considered for this programme, you must be nominated by your home university in the DTU Exchange Student system. Once you have been nominated, you must complete your nomination by uploading the following documents:

- Grade transcripts (in English) including an official description of the grading scale
- Documentation proving that you have passed one of the above English language tests

### **Step 2: Application**

To apply, please open the link "Apply now", fill out the online application form, and attach all your materials in English as PDF files. The files must include:

- A CV including information about your education, relevant research experience, language skills, and other skills relevant to the internship position
- A motivated cover letter (max. 1 page)

Your complete online application must be submitted no later than 15 September 2026 (23:59 Danish time).

We look forward to receiving your application.

*DTU is one of Europe's leading elite technical universities. Through research and education at an international top level, we create solutions to the major societal challenges of our time and help secure Europe's global leadership in sustainable technological development. Since Hans Christian Ørsted founded DTU almost 200 years ago, our mission has remained the same: We develop and create value through the natural and technical sciences for the benefit of society. DTU has 13,800 students, 1,600 PhD students, and 6,500 employees. We work in an international environment and have an inclusive, stimulating, and informal work culture. DTU has campuses in all parts of Denmark and in Greenland and collaborates with the best universities around the world.*

**Application deadline**

16 September 2026

**Study level**

Bachelor level or equivalent

**Job Category**

Engineering

**Related tags**

DTU Global Top Student Programme