Three Doctoral Researchers in Machine-Learning-Driven Atomistic Simulations
Aalto University

Job Title	Three Doctoral Researchers in Machine-Learning-Driven Atomistic Simulations
Department	T105 Chemistry and Materials
Institution	Aalto University , , Finland
Date Posted	Jul. 7, 2025
Application Deadline	Open until filled
Position Start Date	Available immediately
Job Categories	Graduate Student
Academic Field(s)	Computer Engineering Computer Science
Job Website	https://aalto.wd3.myworkdayjobs.com/aalto/job/Otaniemi-Espoo-Finland/Three-Doctoral-Researchers-in-Machine-Learning-Driven-Atomistic-Simulations_R43701-4
Apply By Email	

Job Description

Aalto University is where science and art meet technology and business. We shape a sustainable future by making research breakthroughs in and across our disciplines, sparking the game changers of tomorrow and creating novel solutions to major global challenges. Our community is made up of 120 nationalities, 14 000 students, 400 professors and close to 5000 faculty and staff working on our dynamic campus in Espoo, Greater Helsinki, Finland. Diversity is part of who we are, and we actively work to ensure our community’s diversity and inclusiveness. This is why we warmly encourage qualified candidates from all backgrounds to join our community.

The School of Chemical Engineering ([url=https://www.aalto.fi/en/school-of-chemical-engineering]CHEM School) is one of the six schools of Aalto University. It combines natural sciences

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and engineering in a unique way. We are now looking for:

Three (3) Doctoral Researchers (PhD students) in Machine-Learning-Driven Atomistic Simulations

The Data-driven Atomistic Simulation (DAS) group, led by Prof. Miguel Caro at the Department of Chemistry and Materials Science, Aalto University, is looking for three PhD students to join cutting-edge research projects in atomistic modeling, machine learning, and computational materials science. Positions 2 and 3 are under the direct supervision of Prof. Caro as part of various research projects while Position 1 is under direct supervision of Dr. Rina Ibragimova within her recently granted Research Council of Finland Fellow project SpaceML. All three doctoral students will be fully integrated within the DAS group, a vibrant research environment whose core expertise is the development of machine-learning-infused atomistic modeling techniques beyond the state of the art and their application to study important problems in chemistry, physics and materials science. The group has access to state-of-the-art supercomputing facilities (like LUMI) and is very well integrated within the scientific community internationally. More about our activities: [url=https://miguelcaro.org/]https://miguelcaro.org. Informal inquiries about the positions can be directed to Miguel Caro (miguel.caro@aalto.fi) for positions 2-3 and Rina Ibragimova (rina.ibragimova@aalto.fi) for position 1. If your question is relevant to all 3 positions, feel free to email both. Please, read the description below in full before directly contacting us by email.

The three positions are fully funded and focus on the following research problems: *
Position 1 is integrated within the project “Simulation of complex organics in astrophysical environments using machine learning (SpaceML)”, funded by the Research Council of Finland and supervised by Academy Fellow Dr. Rina Ibragimova within Prof. Caro’s group. The project focuses on investigating the formation and destruction of organics in the circumstellar environment using machine learning and computational chemistry. *
Position 2 will seek to develop a new computational method combining atomistic modeling with experimental microscopy as an extension of our group’s original modified Hamiltonian formalism. This new method will be used to understand the atomistic structures of complex materials, like carbonized biomass for energy applications, across scales. *
Position 3 will develop and utilize atomistic machine learning methods to study structural transformations taking place at the atomic scale via accelerated simulation. The new methods will be used to study pyrolysis and relaxation processes in glasses.

Your responsibilities will include: *
Performing scientific research as instructed by the supervisor(s). *
Documenting your progress and producing scientific texts and figures leading to the publication of articles in peer-reviewed journals. *

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Generating and documenting code and datasets. *
Collaborating with international experts, both computational and experimental. *
Fulfilling the requirement of the Doctoral Programme in Chemical Engineering (graduation typically in four years). More info and eligibility criteria: [url=https://www.aalto.fi/en/study-options/doctoral-programme-in-chemical-engineering]https://www.aalto.fi/en/study-options/doctoral-programme-in-chemical-engineering.

For all the positions, a small number of educational credits need to be completed before graduation. The target time for graduation is 4 years. Additional minor tasks may include teaching assistant duties, help in event organization, etc. The PhD students will contribute to the development of the TurboGAP code ([url=https://turbogap.fi/]https://turbogap.fi) in collaboration with existing members of the Caro group and external collaborators. All the positions include collaboration with international experts, both computational and experimental.

Position-specific job descriptions are as follows:
Position 1: This positions involves: 1) Developing machine learning interatomic potentials for modelling organics under astrophysical conditions (taking into consideration chemical reactivity and UV irradiation effects); 2) Exploring new methods for the development of ML infrared spectra prediction tools; 3) Performing high-throughput calculations of organics destruction/synthesis process in astrophysical environments; 4) Collaborating with experimentalists to benchmark our results; 5) Preparing research manuscripts for submission in top-tier journals. SpaceML is a multidisciplinary collaborative project, where we will cooperate with astrophysicists and material scientists from Institute of Astrophysics of the Canary Islands and The Material Science Institute of Madrid, to explain astrophysical observations from James Webb and Spitzer space telescopes and build a unified computational framework capable of capturing complex interactions in organic matter for use across different research fields.

Positions 2-3: These positions include a fair amount of method development and implementation, in addition to application to study problems in materials science. The method development workflow typically involves literature survey, followed by pen/paper/blackboard brainstorming, followed by implementing a prototype solution in Python (and several iterations of going back to the blackboard to fix various issues). A working prototype solution is eventually implemented in parallel (MPI-based) Fortran into the TurboGAP code for high-performing production simulations on a supercomputer. At this point, the task is to study the materials problem at hand with existing and own (including existing and the newly developed) computational tools, including benchmark against experimental data and/or direct integration of experimental data into the simulation pipeline (see [url=https://doi.org/10.1021/jacs.4c01897]https://doi.org/10.1021/jacs.4c01897). The new Fortran implementations will further be ported to GPU, either by you (if you are interested in this) or by our

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collaborators at the CSC supercomputing center. For position 2, the method development will include machine learning based image recognition/processing techniques to enable computational microscopy and experimental matching. For position 3, the method development will include the modification of existing optimization procedures to explore the potential energy surface of materials in search of transition states and structural transformations using existing and newly developed atomistic machine learning techniques. Our network of collaborators for these PhD projects includes international partners Albert Bartók (Warwick), Xi Chen (Lanzhou), Gábor Csányi (Cambridge), Volker Deringer (Oxford), Dorothea Golze (Dresden) and Hannes Jónsson (Iceland), in addition to local experimental and computational experts from Aalto University, VTT and CSC.

To succeed in this role, you should have: *
A Master’s degree (or equivalent*) in Chemistry, Physics, Materials Science, Mathematics, Computer Science, or a related field. (*You are required to have a degree that would allow you to enroll for a PhD program in the granting institution, e.g., a 1st hons BSc in the UK is also eligible.) *
Prior programming experience, especially with Python. While you are not expected to be an expert programmer, some hands-on experience in programming is mandatory for all 3 positions. Experience with compiled languages (C/C++/Fortran) and/or GPU programming is a strong advantage for positions 2-3. Note that it will be entirely possible to develop the more advanced programming skills during the doctoral studies. *
A strong interest in atomistic simulations, machine learning, and scientific method and software development. *
Proficiency in English (written and spoken). *
(Preferred) Experience with any of the following: *
Electronic structure software (e.g., VASP, GPAW, FHI-aims). *
Molecular dynamics packages (e.g., LAMMPS, GROMACS). *
Machine learning interatomic potentials (e.g., GAP, MACE, ACE). *
Machine learning libraries and frameworks such as Scikit-learn, TensorFlow, or PyTorch. *
If you have experience with other types of modeling tools (e.g., FEM), please state it in your cover letter.

Research experience (e.g., BSc/MSc theses, internships) is expected, but publications are not required. Please briefly describe your past research experience and role in any projects or publications in your cover letter. If you have scientific publications, briefly explain in your cover letter how you contributed to them. At the PhD student level, we are more interested in your ability to do the planned work than a list of publications.

If you feel you are interested and qualified for the position but are concerned about not fulfilling all the criteria, still feel free to apply. Take a look at

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[url=https://www.forbes.com/sites/adunolaadeshola/2025/01/30/worried-youre-not-qualified-for-the-job-you-want-apply-anyway-heres-how/]this article in Forbes.

What we offer / key employment details
Aalto’s Department of Chemistry and Materials Science is a leading research environment in Finland for computational chemistry and materials science, with four groups specializing in different branches (Soft Materials Modelling, Computational Chemistry, Inorganic Materials Modelling, and Data-driven Atomistic Simulation).

The position offers a starting gross salary of 3075 euros per month. The appointment will be made by a fixed-term contract, initially for one year during which you will apply for the study right in doctoral studies, with extensions available up to four years. The role also includes occupational health benefits and access to Finland’s comprehensive social security system. The starting date for the position is in Fall 2025, but the exact date can be agreed with the selected candidate.

How to apply
Please submit your application through our online system no later than 31 July 2025, using the “Apply Now!” button below. Include the following documents in English (PDF format): *
Cover letter (max 1-2 pages): Include your name and email. Briefly motivate your interest in the position and explain how/to what extent you fulfill the requirements. Include the names, positions and emails of 1-3 referees who could provide a letter of reference or recommendation upon request by us. Briefly mention any prior research experience you may have. If you are interested only in one of the advertised positions, you can state which one here. You can also rank the advertised positions according to interest if you prefer one of them but are potentially also interested in the others. Please, do not use ChatGPT or similar tools to prepare your cover letter for you. *
Curriculum vitae: personal and academic information, list of skills, projects, etc. Lying on your CV is immediate grounds for disqualification. If you are invited for an interview, you will be asked about information provided here. *
Copy of your Master’s degree certificate and a transcript of your studies.

The top candidates will be invited for a Zoom interview soon after the deadline.

Contact: *
For Position 1: Dr. Rina Ibragimova - rina.ibragimova@aalto.fi *
For Positions 2-3: Prof. Miguel Caro - miguel.caro@aalto.fi
If your question relates to all three positions, you are welcome to contact both.

Applications sent via email will not be considered; only submissions through the “Apply Now!” button

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are accepted.

Please note: Aalto University’s employees should apply for the position via our internal HR system Workday (Internal Jobs) by using their existing Workday user account (not via the external webpage for open positions). If you are a student or visitor at Aalto University, please apply with your personal email address (not aalto.fi) via [url=https://www.aalto.fi/en/careers-at-aalto]Aalto University open positions.

Aalto University is committed to equality and diversity in our work community. We encourage qualified applicants from all backgrounds to apply and join our innovative research team.

About Finland
Finland is a great place for living with or without family - it is a safe, politically stable and well-organized Nordic society. Finland is consistently ranked high in quality of life and was just listed again as the happiest country in the world: [url=https://worldhappiness.report/news/its-a-three-peat-finland-keeps-top-spot-as-happiest-country-in-world/]https://worldhappiness.report/news/its-a-three-peat-finland-keeps-top-spot-as-happiest-country-in-world/. For more information about living in Finland: [url=https://www.aalto.fi/en/careers-at-aalto/why-finland]https://www.aalto.fi/en/careers-at-aalto/why-finland

Contact Information

Contact

Finland