



PhD-Student-in-molecular-modelling-and-machine-learning

Apply now

Context: the PHYMOL project and AMS

Avant-garde Materials Simulations (AMS) is in charge of the [DC5 package](#): AI/ML assisted parameter generation for an ab-initio-grade force field covering all mainstream organic chemistry.

Duration: 36 months

Background: Tailor-made Force Fields (TMFFs), i.e. parametric force fields fitted fully automatically from scratch to ab initio data, have strongly contributed to AMS' success in the field of [Crystal Structure Prediction](#) (CSP) and are also available for use in third-party software through the Force Field Factory module in [AMS' GRACE code](#). Because of their unique speed-accuracy compromise, parametric force fields will continue to play a role even when Machine Learning (ML) force fields will become generally applicable.

Objectives: The goal of the project is twofold: improve the mathematical framework of tailor-made force fields to further approach ab initio accuracy and reduce the CPU time requirements of the parameterization procedure by means of modern Artificial Intelligence (AI) and ML tools.

Supervisor: Dr. Marcus A. Neumann (AMS)

Co-supervisor: Prof. Alexander Tkatchenko (University of Luxemburg)

Mentor: Dr. Alston J. Misquitta (Queen Mary University of London)

Further information: [More on Phymol](#)

Note: Another Ph.D student of the PHYMOL project, Rony Letona (DC9), also works at AMS and is registered at the University of Luxemburg with the same co-supervisor and mentor.

Why apply to PHYMOL?

PHYMOL is a [doctoral network](#) that combines training and research in almost equal parts. Further, the network is built around a community of leading researchers and all doctoral candidates will be part of this community through secondments, training schools, PHYMOL events, and conferences. Here's what you could stand to get from PHYMOL:

- The chance to participate in workshops and conferences.
- To interact with international laboratories and industrial partners.
- To perform cutting-edge research in a community of excellent researchers, both academic and industrial.
- To be involved with cool science that combines fundamental physics, chemical physics, models, machine-learning, and applying to challenging problems.
- To be able to travel to partners, conferences, laboratories.

AMS 's flagship product [GRACE](#) has been developed with and for our customers for over twenty years. From the early days up until today, we have been tightly connected to the experimental departments of some large pharmaceutical companies, embracing their problems as ours.

We have pioneered and become the world-leader of organic [Crystal Structure Prediction](#).

Through the [PHYMOL](#) project we intend to strengthen the ties with leading academic groups in our field.

Our offices are located in [Freiburg](#) (Merzhausen), Germany, on the border of the [Black Forest](#). The city has a rich student life with a variety of places to unwind after work. The residential areas offer [green](#), calm surroundings that are ideal for healthy lifestyles and families. Close to France and Switzerland, the Black Forest is one of Germany's most touristic regions known for the beauty of its lakes and landscapes. In the wintertime the region offers good opportunities for alpine and cross-country skiing.

Your responsibilities

You will drive and execute a project entitled “AI/ML assisted parameter generation for an ab-initio-grade force field covering all mainstream organic chemistry”.

Parametric force fields offer a unique speed/accuracy compromise for molecular modelling applications: To extend the usefulness of parametric force fields, you will:

1. Improve the accuracy of the force field
2. Accelerate the force field parameter generation

To improve the accuracy, the you will first implement, parametrize and test potential energy functions to describe the coupling of intra- and intermolecular interactions with a special focus on capturing the change of vibrational frequencies induced by the environment. During this phase you will get to know AMS' infrastructure for generating, handling and using both ab initio reference data and force field parameters derived from these data.

To reduce the CPU-time burden in parametrizing TMFFs, the you will explore various avenues potentially including but not limited to 1) Acceleration of the global parameter optimization by replacing the all-parameters-all-data minimizer by a stochastic decent approach, 2) pre-parameterization for certain classes of compounds (solvents, co-formers, etc.), 3) artificial Intelligence (AI) and ML approaches to learn parameters from the results of previous force field parameter optimizations and 4) training of deep neural networks to generate force field parameters directly trained on reproducing ab initio energies and forces, 5) using third-party neural networks to obtain electrostatic multipoles and polarizabilities combined with a local ML model capturing intramolecular interactions.

You will carry out software development in both C++ and Python. Calculations will be run on one of AMS' high-throughput in-house LINUX clusters featuring several thousands of cores. You will meet several times per week with your supervisor at AMS to decide on short-term priorities and once per month with the software development and contract research teams to brainstorm about problem solution strategies and to identify permanent staff members best suited to train you on the required skills.

You will register at the University of Luxemburg as a Ph.D student, spend several months there in Prof. Tkatchenko's group to be trained on ML and ultimately receive your degree from the University of Luxemburg.

Your profile

Soft skills: do you share our vision and values?

- You care about reducing your carbon footprint at work and Ethics in Science
- Intercultural awareness: you enjoy having to cooperate with very diverse business logics and work cultures.
- You are rigorous, precise and solution-oriented
- You can execute complex sub-projects independently
- You have a genuine interest in the development of efficient computer algorithms
- You are concerned by gender equality at work and accept guidance by senior colleagues

Hard skills: do you bring in...?

- Excellent math skills
- Good programming skills (ideally in C++ and Python)
- Physical and mathematical intuition
- Previous experience with ML/AI tools would be a plus

Education

Master in computer science, physics, chemistry, or a related field.

What we offer: a workplace to shape your future

We are a small family business with short communication paths.

We aim to provide a professional environment in which people from all over the world at different stages of their lives can find the work-life balance that suits them.

Specifically related to the PHYMOL project, you will:

Be supervised by Dr. Dzmitry Firaha, co-supervised by Prof. Alexander Tkatchenko from the University of Luxemburg and mentored by Alston Misquita from Queen Mary University of London.

Obtain a PhD from the University of Luxemburg

Have the opportunity to spend 6 months in Prof. Tkatchenko's group in Luxemburg where you will receive training on machine learning.

Because we care about our employees, our customers' needs, scientific progress and the planet, working at AMS does have a meaning.

- Flexible work time management around core hours
- Free organic coffee & teas, terraces for lunches and breaks
- Resilient, organic garden with a planter where employees can grow their own fruits and vegetables
- A quiet workplace with the quality of a living space (not open plan offices)
- Job specific training
- Yearly: 28 days paid leave (full time based) + about 10 days public holidays
- Equal opportunity policy
- Help with settling in if you are located outside Germany

What about recruitment for this PHYMOL project?

Find all details about the recruitment for the PHD position :

<https://www.phymol.eu/recruitment.php>

Avant-garde Materials Simulation Deutschland is an [equal opportunities](#) recruiter: your application is welcome regardless of your age, gender, ethnic origin, disabilities or religion/beliefs.

Sharing a [common mindset and work Ethics](#) is the key to a diverse and happy [Team!](#)

Apply now

People at AMS

Discover Avant-garde Materials Simulation Deutschland GmbH.

Sharing a [common mindset at work](#) is the key to a diverse and happy [Team!](#)



Our mindset

- We are addicted to innovation
- Our software is used by many large pharmaceutical companies
- Our customer's problems are our problems
- We are a family business
- We do business to invest in science, not the other way around

Our Business Ethics

- Sustainable development
- Renewable energies
- Soft mobility and CO2 offset for travels
- Low energy consumption
- A culture of respect and openness towards colleagues and partners