

ELEGANCE: machinE LEarning for inteGrated multi-parAmetric eNzyme and bioproCess dEsign

DC12: Development of machine learned coarse grained force fields for computational enzyme design

Organization

Freie Universität Berlin (FUB) – founded in 1948 – is a full university with 15 departments and central institutes offering 170 degree programs across a wide range of subjects. FUB currently has about 33.000 students and 4.000 PhD students. FUB is one of the few German universities that were successful in all three funding lines of the German federal and state Excellence Initiative, thereby receiving additional funding for its institutional future development strategy. In the recent Excellence Strategy research competition run by the German federal and state governments, FUB won four Clusters of Excellence. These interdisciplinary research projects will each be funded for 7 years. Since 2019 FUB is a partner of the Berlin University Alliance, which brings together 4 Berlin Higher Education Institutions to consolidate their strengths and open opportunities for new innovative research. The “Times Higher Education World University Ranking 2023” places FUB among the 100 most renowned universities worldwide. According to the ranking of the Alexander von-Humboldt Foundation, FUB ranks first in Germany with regards to attracting international scholars. FUB has a steady position in Top 10 German Universities in terms of DFG-Grants.

The doctoral candidate (DC) will work in Clementi's group in the Department of Physics of FUB. Clementi's group develops and applies novel approaches to simulate long timescale dynamics of complex macromolecular systems at multiple resolutions, by means of simulation, statistical physics, and machine learning. The group has dedicated space that has been recently renovated, administrative support, and access to large computational infrastructures.

Roles and responsibilities

The PhD will be carried out in 3 years (with possibility of +1 year extension) at FUB under the supervision of Dr. Cecilia Clementi. Within this time, it is expected that two research stays (6 months and 3 months) will be conducted, the first in an academic group in Spain and one industrial stay in Denmark. The Horizon Europe Marie Skłodowska-Curie Action (MSCA) doctoral network (DN) project starts in January 2026. The date of recruitment and state of the PhD project is planned latest by December 2026. Your PhD degree will be awarded based on successful completion of the research work at FUB. You will also be required to participate in the training events organized by the DN and you are expected to contribute with the dissemination of your PhD results via social media and public engagement.

The PhD project will focus on:

- Development of a fully transferable machine-learned coarse grained (MLCG) protein force field for the study of the slow ($> \text{ms}$) dynamics of large (> 500 residue) proteins and protein complexes
- Testing and implementation of long-range interaction architectures in the MLCG force field
- Long timescale simulations and analysis of specific enzymes with the developed MLCG force-field
- Design of enzymes by considering their dynamics over multiple timescales
- Integration of the developed tools in the ELEGANCE network pipeline

Main supervisor: Cecilia Clementi, Freie Universität Berlin, Berlin, Germany

Co-supervisor 1: Sílvia Osuna, University of Girona, Spain

Co-supervisor 2: Peter Hallin, Novozymes, Bagsværd, Denmark

Qualifications:

- MSc in Physics or comparable degree
- Experience with biomolecular simulation
- Experience with deep learning, in particular graph neural network architectures
- Excellent English proficiency in written and oral form
- Excellent communication skills for working within an interdisciplinary research team
- Strong analytical skills and ability to work independently

Preferred qualifications but not mandatory:

- Experience with molecular dynamics codes like OpenMM, Gromacs, etc.
- Experience with ML tools in Python such as pyTorch
- Experience with protein software tools like AlphaFold3, Boltz2, PyMOL, Chimera, etc.
- Interest in advanced computational methods to improve and understand protein function
- Interest in entrepreneurship to make a positive impact on planetary and human health

Conditions of employment

You must have a two-year master's degree (120 ECTS points) or a similar degree with an academic level equivalent to a two-year master's degree.

Approval and Enrolment

The scholarship for the PhD degree is subject to academic approval, and the candidate will be enrolled in one of the general degree programmes at FUB. For information about our enrolment requirements and the general planning of the PhD study programme, please see [FUB's rules for the PhD enrolment](#)

We offer

FUB is a leading technical university globally recognized for the excellence of its research, education, innovation and scientific advice. We offer a rewarding and challenging job in an international environment. We strive for academic excellence in an environment characterized by collegial respect and academic freedom tempered by responsibility.

Salary and appointment terms

The preferred starting date is 1st June 2026 or according to mutual agreement. The position is full time. The monthly salary will be a lump sum in the range of 3.753,00 EUR to 4.273,00 EUR (gross salary before taxes, insurance, etc.) depending on family status. The period of employment is 3 years, with potential extension of +1 year upon available funding.

Further information

Further information may be obtained from Cecilia Clementi: s.hartmann-rolke@fu-berlin.de

Website about MSCA doctoral network ELEGANCE: <https://elegance.dtu.dk/>

Google Scholar profile: <https://scholar.google.de/citations?user=0na1SpQAAAAJ&hl=en>

More information about Clementi's group: <https://www.physik.fu-berlin.de/en/einrichtungen/ag/ag-clementi>

If you are applying from abroad, you may find useful information on working in Germany and at FUB at [FUB - Welcome service](#).

Application procedure

Your complete online application must be submitted no later than **December 15th, 2025 (23:59 German time)**. Applications must be submitted as **one PDF file** containing all materials to be given consideration.

To apply, please assemble **all your materials in English in one PDF file**. The file must include:

- A letter motivating the application (cover letter)
- Curriculum vitae
- Grade transcripts and MSc diploma (in English) including official description of grading scale

You may apply prior to obtaining your master's degree but cannot begin before having received it.

Applications received after the deadline will not be considered.

All interested candidates irrespective of age, gender, disability, race, religion or ethnic background are encouraged to apply.

Please submit your application by email to: s.hartmann-rolke@fu-berlin.de