



Conducting research for a changing society: This is what drives us at Forschungszentrum Jülich. As a member of the Helmholtz Association, we aim to tackle the grand societal challenges of our time and conduct research into the possibilities of a digitized society, a climate-friendly energy system, and a resource-efficient economy. Work together with around 7,500 employees in one of Europe's biggest research centres and help us to shape change!

Molecular machine learning harnesses the power of foundation models to revolutionize protein dynamics and design, small molecule property prediction, and protein function prediction. By integrating state-of-the-art machine learning techniques with molecular biology and computational chemistry, we aim to push the boundaries of innovation in these fields. This role offers the opportunity to work on impactful projects at the intersection of artificial intelligence and molecular sciences, contributing to breakthroughs in drug discovery, biotechnology, and molecular engineering.

In projects financed by the Helmholtz Association, we aim to take the field of molecular foundation models to the next level. The potential applications are transformative, including dynamic enzymes, programmable molecular machines, smart therapeutics, sustainable materials, and next-generation biotechnologies.

The subinstitute IBG-4 – Bioinformatics develops and implements algorithms and tools from the fields of machine learning, molecular simulation and modeling, to address molecular questions in bioeconomy.

Join our team to the next possible date as

Postdoc - Molecular Machine Learning with Foundation Models

Your Job:

We are seeking highly motivated postdoctoral researchers to join these projects.

If you are passionate about protein dynamics and design, protein function prediction, small molecule property prediction, modern artificial intelligence methods, molecular dynamics, and interdisciplinary research, this is your chance to be part of an exciting journey at the forefront of science and technology.

- Development of cutting edge foundation models for protein design, small molecule property prediction, or protein function prediction
- Data generation and curation, including molecular simulation and genomic

The job will be advertised until the position has been successfully filled. You should therefore submit your application as soon as possible. We look forward to receiving your application via our

Online-Recruitment-System!

Questions about the vacancy?

Get in touch with us by using **our contact form**.

Please note that for technical reasons we cannot accept applications via email.

www.fz-juelich.de

approaches

- Application of the modeling approaches in relevant downstream tasks
- Co-development of high-performance computing AI training codes for the first European Exascale Supercomputer JUPITER
- Engagement in national and international ML/DL communities and the Helmholtz Foundation Model initiative
- Present research results at scientific meetings, conferences, and as scientific publications

Your Profile:

- A Master's degree and an excellent PhD degree in Biochemistry, Chemistry, or a related Molecular Science
- Proven Track Record in Machine Learning, Molecular Simulations, Chemoinformatics, Statistical Physics, Genome Annotation, and/or related fields
- Practical experience with High Performance Computing Systems as well as parallel/distributed programming
- Very good command of written and spoken English
- Your experience should be documented in research papers and Open Source code projects
- Self-motivated personality, curiosity about working in a multi-disciplinary team environment on scientifically challenging problems

Our Offer:

We work on the very latest issues that impact our society and are offering you the chance to actively help in shaping the change! We support you in your work with:

- Work on frontiers of scientific and technological challenges with access to cutting-edge and unique supercomputing systems
- Scientific work embedded in a vibrant community of experts in Molecular Modeling and Simulations, Machine Learning, and lab research
- An exciting working environment on an attractive research campus, located between the cities of Cologne, Düsseldorf, and Aachen
- Full-time position with the option of slightly reduced working hours and 30 days of annual leave
- Flexible working hours and various opportunities to reconcile work and private life
- Targeted services for international employees, e.g., through our International Advisory Service

In addition to exciting tasks and a collaborative working atmosphere at Jülich, we have a lot more to offer:

<https://go.fzj.de/benefits>

We offer you an exciting and varied role in an international and interdisciplinary working environment. The position is for a fixed term of 2 years, with possible long-term prospects. Salary and social benefits will conform to the provisions of the Collective Agreement for the Public Service (TVöD-Bund), pay group EG 13, depending on the applicant's qualifications and the precise nature of the tasks assigned to them. All information about the Collective Agreement for the Public Service (TVöD-Bund) can be found on the BMI website: <https://go.fzj.de/bmi.tvloed>. The monthly salaries in euros can be found on page 66 of the PDF download.

We welcome applications from people with diverse backgrounds, e.g. in terms of age, gender, disability, sexual orientation / identity, and social, ethnic and religious origin. A diverse and inclusive working environment with equal opportunities in which everyone

can realize their potential is important to us.

