



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!

The Institute of Neuroscience and Medicine - Computational Biomedicine (INM-9, <https://www.fz-juelich.de/en/inm/inm-9>) uses and develops high performance computing-based multiscale approaches to investigate key molecular events for neuronal function and dysfunction. INM-9 is also part of relevant European initiatives like the joint doctorate program STIMULATE (<https://stimulate-ejd.eu/stimulate-ejd.eu/index.html>) and the Center of Excellence BioExcel (<https://bioexcel.eu/>) to support the use of high-performance computing and high-throughput computing in biomolecular research. Recent advances in machine learning and protein structure prediction, particularly AlphaFold, have opened new avenues for modeling such transitions and integrating structural and dynamical information. In this project, deep learning models will be developed to guide enhanced sampling simulations and uncover the molecular determinants underlying protein activation and allosteric regulation.

We are offering a

PhD Position - Simulations and machine learning applied to proteins

Your Job:

- Modeling and characterization at molecular level of selected biological processes by performing classical molecular dynamics, and employing enhanced sampling methods and machine learning techniques
- Writing and submitting computational proposals to obtain the computational resources required to accomplish the project
- Engage in the international simulation community
- Publishing the results of this project in international journals and presenting them at international meetings and conferences

Your Profile:

- Excellent university degree (Master) in physics, chemistry, bioinformatics, applied mathematics or computer science

We look forward to receiving your application until 10.11.2025 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

- Experience with UNIX-like operating systems
- Mathematical and programming skills (Python, Machine Learning)
- Basic understanding of molecular forces and structures
- Excellent knowledge of written and oral English
- Interactive person with good communication skills
- Used to work in international teams
- Ideal prior knowledge on MD simulations

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:

- **TEAM & ENVIRONMENT:** You will work in a motivated team with an international and interdisciplinary focus – at one of the largest research institutions in Europe
- **RESEARCH & INFRASTRUCTURE:** You will have access to excellent scientific and technical facilities for your work. A Doctoral degree conferred by RWTH Aachen University
- **NETWORKING & EXCHANGE:** You will participate in (international) conferences and project meetings and actively build your scientific network
- **SUPERVISION & SUPPORT:** We will accompany your doctoral studies with continuous, expert guidance from your academic supervisor
- **WORK-LIFE BALANCE:** We offer a part-time position with 19,5 hours per week with flexible working hours to help you balance your professional and personal life. You also have the option of flexible working (in terms of location), which is generally possible after consultation and in line with upcoming tasks and (on-site) appointments
- **VACATION:** You will receive 30 days of vacation
- **KNOWLEDGE & DEVELOPMENT:** Your professional development is important to us – we support you specifically and individually e.g., through training and networking opportunities specifically for doctoral candidates (JuDocS): <https://go.fzj.de/JuDocs>
- **FAIR REMUNERATION:** Depending on your qualifications and assigned responsibilities, you will be classified according to pay group 13 (70%) of the TVöD-Bund. Additionally, you will receive a special payment (“Christmas bonus”) amounting to 60% of one month’s salary. All information about the TVöD-Bund collective agreement can be found on the BMI website (pay scale table on page 66 of the PDF download): <https://go.fzj.de/bmi.tvöed>
- **FIXED-TERM:** The position is limited to 3 years
- **SUPPORT FOR INTERNATIONAL EMPLOYEES:** Our International Advisory Service makes it easier for international employees to get started

In addition to exciting tasks and a collegial working environment, we offer you much more: <https://go.fzj.de/benefits>

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.

The following links provide further information on diversity and equal opportunities: <https://go.fzj.de/equality> and on specific support options: <https://go.fzj.de/womens-job-journey>