Shaping change: this is what drives us at Forschungszentrum Jülich. As a member of the Helmholtz Association with some 7,600 employees, we conduct interdisciplinary research into a digitalized society, a climate-friendly energy system, and a sustainable economy. We focus on the natural, life, and engineering sciences in the fields of information, energy, and bioeconomy. We combine this with expertise in high-performance computing and artificial intelligence using unique scientific infrastructures.

The Bioinformatics Division of the Institute of Biological and Geosciences - Bioinformaticsc(IBG-4) processes and develops methods and algorithms to achieve a fundamental understanding of high-dimensional data and processes in the bioeconomy in particular. Bioinformatics at Forschungszentrum Jülich plays a leading role at the international level, for example in the field of plant and microbial data management, in the evaluation of new methods of genome analysis, in the integration, interpretation, and visualization of high-dimensional omics data from the field of bioeconomics, and in the modeling, simulation, and engineering of biomolecular systems, including enzymes.

Apply your data science skills to real-world challenges!
At the Helmholtz School for Data Science in Life, Earth and Energy (HDS-LEE), we train the next generation of data scientists to tackle key global issues in domain sciences such as life, earth or energy. Learn more at www.hds-lee.de Institute specific promise here.

We are looking to recruit a

PhD position - Molecular simulation and machine-learning for predictive chromatography modeling with CADET - within the HDS-LEE graduate school

Your Job:
Chromatography modeling, while crucial for modern bipporcess development, still heavily relies on empirical determination of key model parameters. By combining protein structure descriptors, molecular simulations, and machine learning, this PhD project seeks to predict ion-exchange isotherm parameters directly from molecular properties. These predictions will be integrated into the open-source CADET simulation framework, enabling fully predictive process simulations without extensive experimental calibration.

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

Embedded in the Helmholtz Graduate School for Data Science in Life, Earth and Energy (HDS-LEE), the project offers an interdisciplinary research environment at the interface of bioengineering, computational biophysics, and data-driven modeling, with strong links to open-source software development and industrially relevant applications. Tasks include:

- Development of molecular descriptors from protein structures and simulations
- Design and training of QSPR and machine learning models to predict ion-exchange isotherm parametersIntegration of predicted parameters into the CADET chromatography simulation framework
- Simulation and analysis of batch and gradient elution processes using predictive isotherms
- Curation and analysis of experimental chromatography data for model training and validation
- Collaboration with experimental and industrial partners
- Dissemination of results through high-quality publications and open-source software contributions

Your Profile:

- Master's degree in chemical engineering, biotechnology, computational biophysics, bioinformatics, data science, or a closely related discipline with a strong academic record
- Genuine interest in data-driven and physics-based modeling, molecular simulations, and their application to bioprocesses and bioseparations
- Proficiency in at least one programming language, preferably Python; experience with scientific computing, numerical modeling, or machine-learning frameworks is an asset
- Strong analytical skills with a solid understanding of data evaluation, modeling, and interpretation of complex datasets
- Ability to work independently as well as collaboratively in an interdisciplinary and international research environment
- Very good written and oral communication skills in English; knowledge of German is beneficial but not required
- High motivation for academic development, demonstrated by academic transcripts and references, and interest in publishing and presenting scientific results

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 offer ideal conditions for you to complete your doctoral degree:

- Outstanding research environment and infrastructure: The position is embedded at Forschungszentrum Jülich (FZJ), one of Europe's largest interdisciplinary research centers, offering access to world-class computational resources (HPC), state-of-the-art research software, and close integration with experimental and modeling groups across institutes and Helmholtz programs.
- Structured doctoral training and international visibility: The PhD candidate will be part of the HDS-LEE graduate school, benefiting from a structured qualification program, dedicated mentoring, transferable-skills training, and funding for international conferences, research stays, and networking within the Helmholtz Association.
- Unique combination of science-to-impact opportunities: The project combines molecular biophysics, machine learning, and industrially relevant bioprocess modeling with strong links to open-source platforms (e.g., CADET) and academic–industrial collaborations, offering a rare opportunity to develop skills that

are highly transferable to academia, industry, and large-scale research infrastructures.
- Further development of your personal strengths, e.g. via a comprehensive further training program; a structured program of continuing education and networking opportunities specifically for doctoral researchers via JuDocS, the Jülich Center for Doctoral Researchers and Supervisors: https://www.fz-juelich.de/judocs
- 30 Days of annual leave and flexible working arrangements, including partial remote work
- Targeted services for international employees, e.g. through our International Advisory Service

The position is initially limited to three years, with a planned one-year extension. Pay in line with 75% of pay group 13 of the Collective Agreement for the Public Service (TVöD-Bund) and additionally 60 % of a monthly salary as special payment („Christmas bonus“). Additional compensation beyond the base salary may be possible. All information about the TVöD-Bund collective agreement can be found on the BMI website (pay scale table on page 69 and following of the PDF download): https://go.fzj.de/bmi.tvoed

Further Information: hds-lee@fz-juelich.de

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 for women: https://go.fzj.de/womens-job-journey