At the Institute of Bio- and Geosciences - Biotechnology (IBG-1) we explore the biocatalytic potential of microorganisms and enzymes for sustainable production processes in a bio-based economy.

Typical research projects in our department „Modelling and Simulation“ involve data analysis, model calibration or training, uncertainty analysis, parameter estimation, and experimental design. Model predictions are applied for testing hypotheses and focusing experimental work. We provide our local colleagues and the scientific community with state-of-the-art models, algorithms and software. Current challenges in strain characterization, selection and optimization as well as process analysis and development are addressed in a strongly data-driven, mathematically rigorous fashion in close collaboration between theory, simulation and experiment.

We are looking to recruit a

**PostDoc - Coarse grained modeling of synthetic enzyme cascades**

**Your Job:**
In vitro enzyme catalysis is an effective way of synthesizing industrially valuable chemicals. Carboxylic acid reductases (CARs) are essential enzymes involved in the biosynthesis of aldehydes from carboxylic acids. Therefore, CARs have become attractive catalysts for synthesising valuable aldehyde building blocks. Compared to chemical synthesis, CARs catalyze the one-step reduction of carboxylic acids into aldehydes with little or no over-reduction to alcohols under mild and eco-friendly conditions. Hence, CARs offer a green alternative to aldehyde chemical synthesis. However, reducing carboxylic acids using CARs remains challenging as CARs depend on essential NAD(P)H and ATP cofactors that must be regenerated for self-sufficient and cost-effective processes. The co-expression or addition of auxiliary enzymes and their integration in a multi-enzyme cascade is thus required. To overcome this limitation, we will design locally immobilized multi-enzyme constructs with superior catalytic activity and stability in E. coli compared to unfused enzymes.
The successful candidate will
• Develop coarse-grained (CG) models for CAR and other enzymes of the cascade based on atomistic simulations provided by the project team.
• Run Brownian dynamics simulations of CG model enzymes and their constructs to optimize the overall catalytic activity.

The work will be done in collaboration with Prof. S. Kondrat from the Institute of Physical Chemistry in Warsaw and Stuttgart University.

Your Profile:
• You are an enthusiastic and motivated researcher
• You have a Masters degree and a PhD in physics, chemistry, engineering or related fields
• Ideally you also have experience in Python and molecular simulations
• Good communication skills and a strong interest in multidisciplinary research

Our Offer:
We offer a motivated and interdisciplinary research environment with chemists, biologists, and physicists working closely together. Forschungszentrum Jülich is situated between Cologne and Aachen in Germany and is one of the largest research centres in Europe. 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:
• Comprehensive training courses and individual opportunities for personal and professional further development
• Extensive company health management
• Ideal conditions for balancing work and private life, as well as a family-friendly corporate policy
• Flexible working hours, the option of slightly reduced working hours, and 30 days of annual leave
• A large research campus with green spaces, offering the best possible means for networking with colleagues and pursuing sports alongside work
• Targeted services for international employees, e.g. through our International Advisory Service
• Flexible work (location) arrangements, e.g. remote work to a degree

We offer you an exciting and varied role in an international and interdisciplinary working environment. The position is for a fixed term of 7 months. Salary and social benefits will conform to the provisions of the Collective Agreement for the Public Service (TVöD-Bund), pay group 13, depending on the applicant’s qualifications and the precise nature of the tasks assigned to them.

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 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.