

Applications are invited for a Postdoc position available 1.5.2018 in the Computational Pharmaceutical Chemistry & Molecular Bioinformatics group (Prof. Dr. Holger Gohlke; <http://cplab.uni-duesseldorf.de>) at the Heinrich Heine University Düsseldorf, Germany.

**TOPIC: Computational biotechnology: Energetics and kinetics of substrate channeling in enzyme cascades**

**Background:** Multi-enzymatic cascade reactions, i.e., the combination of several enzymatic transformations in concurrent one-pot processes, offer considerable advantages: the demand of time, costs and chemicals for product recovery may be reduced, reversible reactions can be driven to completion and the concentration of harmful or unstable compounds can be kept to a minimum. However, insufficient transfer of intermediates between the individual enzymes / reaction steps has been recognized as a limiting factor.

In this project, the energetics and kinetics of substrate channeling in enzyme cascades will be investigated by unbiased and biased molecular dynamics simulations. The aim is to gain reliable predictions on how substrate access to the catalytically active centers in enzyme cascades can be optimized by focused mutations and improved immobilization. In addition, modeling and simulation approaches shall provide important clues for optimizing individual cascade enzymes in terms of stability, substrate specificity, and / or stereoselectivity.

The project will be performed in the context of the CLIB (Cluster Industrial Biotechnology; <http://www.clib2021.de/>) Center of Competence “Biotechnology” (CKB), which comprises projects located at four Universities around Düsseldorf, addresses the megatrends resource efficiency, crude materials, and health, and generates an integrated infrastructure for bioeconomy in the state of North-Rhine Westphalia (see also here: <https://www.land.nrw/de/pressemitteilung/elf-projekte-zum-ausbau-von-forschungseinrichtungen-nordrhein-westfalen-sollen-mit>).

**Requirements:** Ideal candidates will have a record of excellence (PhD plus publications in highly visible journals) and a strong background in computational (bio-)chemistry, computational structural biological, molecular simulations, and molecular informatics as well as a high interest in working in an interdisciplinary research field.

Applicants should submit applications (a one-page letter of motivation *why* they are interested in the respective project and *how* they can contribute to the project’s success, a current CV, and contact data of three references) by email to [gohlke@uni-duesseldorf.de](mailto:gohlke@uni-duesseldorf.de) . **Please provide all documents as one PDF file.**

Detailed information about living and studying in Düsseldorf is provided here: <http://www.uni-duesseldorf.de/home/leben-in-duesseldorf.html>