We invite applications for **one PhD student position available immediately** in the Computational Pharmaceutical Chemistry & Molecular Bioinformatics group (Prof. Dr. Holger Gohlke; http://cpclab.uni-duesseldorf.de) at the Heinrich Heine University Düsseldorf, Germany.

TOPIC: Functional state modulation of membrane proteins by dynamic association and dissociation

Background: The central question we intend to investigate within the DFG-funded Collaborative Research Center (CRC) 1208 ("Identity and dynamics of membrane systems – From molecules to cellular function") is how dynamic association and dissociation modulates the functional state of membrane proteins under the condition of conserving their molecular identity.

We will address this question on molecular components central for ethylene perception in plants located at the ER and Golgi membranes (Binder et al., *Annu Plant Rev* 2012; Gohlke and coworkers, *Sci Rep* 2018 & 2019). This (multi)membrane system plays a crucial role in the spatial coordination of dynamic association and dissociation. By molecular simulation and modeling studies at an atomic level closely connected with experimental validation studies, we intend to provide insights into the role and transport of the copper cofactor for ethylene receptor biogenesis and ethylene perception in plants.

As none or only static atomic-level information is available, it is mandatory to develop a conceptual framework of adequate computational approaches for model building and hypothesis generation and high-content experimental platforms to validate and provide feedback. The molecular simulation and modeling studies will be performed by the PhD student in the Gohlke lab. The PhD student will work closely together with scientists of the Groth (http://www.biochemplant.hhu.de/) labs for experimentally validating the established models and generated hypothesis.

Requirements: Ideal candidates will have a record of excellence and a strong background in computational biochemistry/chemistry or structural bioinformatics, a high interest in working in an interdisciplinary collaboration, and profound knowledge in state-of-the-art molecular dynamics simulations (Amber) software, molecular modeling (in particular, protein-protein docking), and QM/MM calculations.

Applicants should submit applications (a one-page letter of motivation *for why* they are interested in the respective project and *how* they can contribute to the project's success, a current CV, credentials, and contact data of three references) by email to 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