

Applications are invited for a PhD student position available 1.1.2018 in the NIC Research Group Computational Biophysical Chemistry (Prof. Dr. Holger Gohlke; [http://www.fz-juelich.de/ias/jsc/EN/AboutUs/Organisation/NICResearchGroupCBC/\\_node.html](http://www.fz-juelich.de/ias/jsc/EN/AboutUs/Organisation/NICResearchGroupCBC/_node.html)) at Forschungszentrum Jülich, Germany.

**TOPIC: Molecular modeling and simulations to improve the GreenRelease technology for plant health**

**Background:** The aim of this project is to make the GreenRelease technology platform (see below) a robust and applicable technology for application in plant health and sustainable agriculture. For this, experimental groups from the fields of polymer chemistry, biotechnology, biochemical plant physiology, and horticulture will work together with our NIC Research Group to achieve this aim. The proof of concept of the GreenRelease technology platform was demonstrated already (see, e.g. 10.1002/anie.v56.26 or 10.1016/j.polymer.2017.03.070). Main advantages of the GreenRelease technology over existing release technologies are the controlled release of compounds over weeks/months, minimized losses due to a high rainfastness, plant compatibility, and tunable biodegradability. Hence, the amount of applied fungicides/herbicides will be reduced significantly and thereby environmental contamination will be minimized (“achieve more with less”). The unique technical application characteristics of the GreenRelease platform are based on properties of microgel containers (200 nm to 10 µm). Microgels are soft porous polymer colloids, which can be loaded with essentially all kinds of compounds and can attach through anchor peptides on plant leaves at ambient temperature by simple spray applications.

Our objective within this project is to *understand interactions between peptides anchoring the microgel containers to leaf surfaces* and to *predict loading and release properties of microgels with respect to selected fungicides* and herbicides to advance the readiness level of the GreenRelease technology. In detail, we will apply rational and (mostly) structure-based technologies for understanding and modulating interactions between peptides, small-molecules, and microgels from a computational perspective. In iterative cycles, our predictions of the computational platform will be tested by the experimental groups. In return, we will make use of experimental results to improve predictions.

**Requirements:** Ideal candidates will have a record of excellence (Master degree in chemistry, biochemistry, biophysics, (structural) biology, or pharmacy) 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 modeling (OpenEye, Schrödinger) and molecular dynamics simulations (Amber) software.

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 [h.gohlke@fz-juelich.de](mailto:h.gohlke@fz-juelich.de) . **Please provide all documents as one PDF file.**

Detailed information about living and working in Jülich is provided here: [http://www.fz-juelich.de/portal/EN/Careers/JuelichAsAnEmployer/OutAndAboutInJuelich/\\_node.html](http://www.fz-juelich.de/portal/EN/Careers/JuelichAsAnEmployer/OutAndAboutInJuelich/_node.html)