HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

Helmholtz

Call for Chinese Applicants Interested in Running for CSC 2021 Fellowship

Helmholtz Centre: Forschungszentrum Jülich GmbH – www.fz-juelich.de
Department/Institute: Institute of Biological Information Processing, Structural Biochemistry (IBI-7) www.fz-juelich.de/ibi/ibi-7/DE/strodel
Supervising scientist: Prof. Dr. Birgit Strodel
Research Field: Computational Biochemistry
Position open for: **Visiting Scholar** **Postdoc: x**
Title of the research: Force-field development for the simulation of protein-protein interactions

More description of research topic:

Protein-protein interactions (PPIs) are the driving force of protein aggregation, which often lead to pathological conditions. Computer simulations have become an increasingly popular research method in the study of protein-protein interactions. Such simulations are based on so-called force fields, providing a physical model of the proteins and their interactions. At present, there are various force field developments for PPIs as research has shown that none of the existing force fields provide perfect models for this problem class. Another problem of protein aggregation is that the length and time scales of this process necessitate so-called coarse-grained force fields as their all-atom counterparts do not allow for long enough simulations to observe protein phase transitions. To overcome these two problems, this project aims to develop a hybrid all-atom/coarse-grained force field for PPIs, thus exploring on a larger scale the systematic effects of PPIs on protein aggregation. For the development of the hybrid force field, machine learning approaches will be applied to efficiently determine the best parameter set.

Specific requirements:

- High level of self-motivation
- Rich expertise in molecular dynamics simulations of proteins
- Experience with Gromacs, NAMD and/or Amber
- Experience with quantum chemistry software like Gaussian or ORCA is beneficial
- Experience in molecular modeling design using VMD, AutoDock and Rosetta.
- Computer skills: Linux, Python, LaTeX required, C/C++ and/or Fortran beneficial

Funding: CSC-scholarships will be increased by hosting institution (600 €/month and costs for health, emergency-call and liability insurance (50 €/month))
Working Place: Forschungszentrum Jülich, Germany (near Cologne)
Earliest Start: September 2021
Language Requirement: Very good knowledge of English language, written and spoken.German language courses are organised in the context of our in-house training program and are free of charge.

Name and Address of the Supervisor: Prof. Dr. Birgit Strodel, Forschungszentrum Jülich, Institute of biological Information Processing (IBI-7), 52425 Jülich, Germany; Email: b.strodel@fz-juelich.de