



PhD Program between the Freie Universität Berlin (FUB) and the China Scholarship Council (CSC)

Open PhD position at FUB for CSC scholarship candidates 2018

Please note: the PhD position is only offered to Chinese PhD candidates for application in the framework of the FUB-CSC PhD Program.

<u>Department/Institute:</u>	Department of Physics
<u>Subject area:</u>	Computational Biophysics
<u>Name of Supervisor:</u>	Prof. Dr. Petra Imhof
<u>Number of open PhD positions:</u>	1
<u>Type of the PhD Study:</u>	Full-time
<u>Project title:</u>	Computational study of enzymatic reactivity

PhD Project description:

Enzymatic reactions are complex transitions, posing a particular challenge for simulation approaches that must embrace both the chemistry as well as the conformational flexibility of the enzymes. Hybrid quantum mechanical/molecular mechanical (QM/MM) methods provide a good compromise for such a task. Allowing the computation of chemical reaction mechanisms in the complete protein model. Such methods are nowadays well established. However, the complex protein environment often renders several mechanisms feasible, the probabilities of which may depend on „exterior“ parameters such as temperature or salt concentration or other spectator molecules, interacting with or binding at allosteric sites, thereby altering the conformational dynamics and hence the reactivity of the protein. In the present project, classical and QM/MM MD simulations will be applied to explore the impact of such factors on the enzymatic specificity (binding the substrate) and its efficiency, i.e. on the preferred reaction pathways.

Language requirements:

IELTS 6.5 or TOEFL 95 ibt.

Academic requirements:

M. Sc. in Physics, Chemistry, or Biochemistry is mandatory. Experience in molecular simulation are required, ideally in both quantum chemistry calculations (electronic structure methods) and molecular dynamics, but at least one of the two. Programming skills in python or java are a clear plus, ability to work on Linux machines is essential.

Information of the professor or research group leader:

The Computational Biophysics group, headed by Prof. Petra Imhof, works at the interface of Physics, Chemistry, Biology and Computer Science. Our Research aims at understanding fundamental processes in biological macromolecules and their interaction by molecular simulations. Website: <http://www.physik.fu-berlin.de/en/einrichtungen/ag/ag-imhof>

Please note: In a first step, the complete application must be submitted to the Beijing Office for evaluation by January 4th, 2018. Please do not contact the professor before. He/She will get in contact with you after having received the complete application via the Beijing Office in January.