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

Open PhD Position at Freie Universität Berlin, offered only to Chinese CSC scholarship candidates 2027

Department/Institute: **Biology, Chemistry, Pharmacy/ Institute for Chemistry and Biochemistry**

Subject area: **Theoretical Chemistry**

Name of Supervisor: **Prof. Dr. Beate Paulus**

Number of open PhD positions: **1**

Type of the PhD Study: Full-time

Project title: **Computational Investigations for the sustainable degradation of PFAS**

PhD Project description:

PFAS are everlasting toxic chemical, where the perfluorination of the aklyl part of the molecule is responsible for their high stability. That makes the degradation difficult as a high amount of energy is necessary to break the CF bonds and therefore many different products (some even more toxic as the PFAS themselves) can be formed. Within the project different catalysts will be investigated computationally for the degration of selected PFAS molecules. For that DFT-based electronic structure methods will be applied together with conformal search workflows to account for the structural diversity of the PFAS. By determination of the transition states a reaction network will be computed. The final goal is the in silico design of the catalyst to achieve non-toxic degradation products, perferable usable as fluorine sources for other reactions.

Language requirements: English

- IELTS: 6,5 oder TOEFL: 95 ibt

Academic requirements:

Master degree in Chemistry or related subjects, with the focus on theoretical and computational chemistry

Information of the professor or research group leader (website, awards etc.):

https://www.bcp.fu-berlin.de/en/chemie/chemie/forschung/PhysTheoChem/agpaulus/index.html
Please note: In a first step, the complete application should be uploaded to the online portal (https://fuberlin.moveon4.de/form/60acfece5d328710e40bdbd5/eng) for evaluation by January 15th, 2027.