



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

**Open PhD Position at Freie Universität Berlin,  
offered only to Chinese CSC scholarship candidates 2025**

**Department/Institute:** BCP, Institute for Chemistry and Biochemistry

**Subject area:** Theoretical Chemistry

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

**Number of open PhD position:** 1

**Type of the PhD Study:** Full-time, no Sandwich

**Project title:** First principle investigations for the interactions of molecules with 2D materials supported by a metal substrate.

### **PhD Project description:**

Within this PhD project first principle investigations mainly at the DFT level will be performed to investigate in the first step the interaction of newly developed 2D materials with metal substrates. That can be for example borophene stabilized by metal surfaces in different structures or graphene deposited on metals to change the electronic structure of graphene. Also semiconducting 2D materials like transition metal dichalcogenides or MXenes are suitable 2D materials for optoelectronic and catalytic applications. The metal support will change their electronic properties and hence their ability to react with selected molecules. To describe this interaction and subsequent chemical reaction on the metal/2D system will be the second part of the thesis. Both adsorption of molecular species on the 2D materials and intercalating systems (molecules on the metal surfaces protected by a 2D material) will be studied. All computational investigations will be in close collaboration with experimental groups, therefore various thermodynamic, kinetic and spectroscopic properties will be calculated to compare directly with measurements.

### **Language requirements:**

- ELTS: 6,5 oder TOEFL: 95 iBT

### **Academic requirements:**

*Master degree in Chemistry, Physics, Material Sciences or related subjects*

*Solid theoretical background in Theoretical Chemistry, i.e. quantum mechanics for electrons*

*Experience with electronic structure software*

**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, 2025