



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

### Open PhD position at FUB for CSC scholarship candidates 2016

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

<b><u>Department/Institute:</u></b>	Department of Biology, Chemistry, Pharmacy/Institute of Chemistry and Biochemistry
<b><u>Subject area:</u></b>	Theoretical Chemistry
<b><u>Name of Supervisor:</u></b>	Prof. Dr. Beate PAULUS (Ms.)
<b><u>Number of open PhD positions:</u></b>	1
<b><u>Type of the PhD Study:</u></b>	Full-time
<b><u>Project title:</u></b>	Quantum theory of symmetry breaking and restauration in atoms and molecules by electric fields and laser pulses

#### **PhD Project description:**

Symmetry breaking is a fundamental and ubiquitous phenomenon in nature [1]. The goal of this PhD project is to discover new ways of symmetry breaking and restauration in atoms and molecules, by means of electric fields and laser pulses, using quantum simulations. This type of symmetry restauration is fundamentally new.

To explain the challenges of the PhD project for a simple example, consider the hydrogen atom in the 2s state. Its isotropic symmetry may be broken by switching on and off a z-polarized electric field. The degeneracy of the 2s and 2p orbitals implies that eventually, the initial 2s orbital is converted into the final anisotropic sp<sub>z</sub> hybrid orbital. The new challenge is to restore isotropic symmetry by means of laser pulses, using the methods of Ref. [2]. Analogous but more ambitious applications are to Rydberg atoms, see e.g. Ref. [3].

Symmetry breaking and restauration in molecules shall be investigated for molecules with symmetric ground states supported by symmetric double well potentials, such as ammonia NH<sub>3</sub>. Symmetry may be broken by a sufficiently strong z-polarized electric field [4]. The task is to design optimal electric fields or laser pulses for restauration of symmetry. This investigation should be extended to more demanding molecules [5].

[1] M. Quack, Adv. Chem. Phys. 157 (2014) 247

[2] C. Liu, J. Manz, Y. Yang, ChemPhysChem 16 (2015) 191

[3] H.-J. Dong, K.-S. Huang, C.-Y. Li, J.-M. Zhao, L.-J. Zhang, S.-T. Jia, Chin. Phys. B. 23 (2014) 093202

[4] C. Liu, J. Manz, Y. Yang, J. Phys. B: At. Mol. Opt. Phys. 48 (2015) 164001

[5] T. Bredtmann, B. Paulus, J. Chem. Theory Comput. 9 (2013), 3026

#### **Language requirements:**

PhD study in English possible, required IELTS 6,5 or TOEFL 95

**Academic requirements:**

Master degree in Theoretical Chemistry or Theoretical Physics.  
Documented experience with quantum simulations of atoms and/or molecules in electric fields and/or laser pulses is seen as an advantage.

**Information of the professor or research group leader:**

<http://userpage.fu-berlin.de/~agpaulus/>

**Please note:**

In a first step the complete application should submit to the Beijing Office for evaluation by January 4<sup>th</sup>, 2016. Please don't contact the professor before. He/She will get in contact with you after having received the complete application in January.