

# Openings

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## TheoChem@RUB: General Information for Applicants (for specific job offers see below):

The University of Bochum (*Ruhr-Universität Bochum*, RUB) is one of the largest Universities in Germany, covering a vast range of fields in the Arts, Science, Engineering, and Medicine. It is member of the German Elite Universities ("Förderlinie Graduiertenschulen der Exzellenzinitiative") as established in fall 2006 based on recommendations of an independent international review panel. RUB is located at the heart of the Ruhr Area (*Ruhrgebiet*), a vibrant metropolitan complex with about nine million inhabitants. The region offers an unusually broad range of cultural and recreational attractions which are easily accessible by the very efficient public transport network.

The Department of Chemistry and Biochemistry (*Fakultät für Chemie und Biochemie*) at RUB is one of the largest faculties on campus. Therein, the Center for Theoretical Chemistry (*Lehrstuhl für Theoretische Chemie*, headed by Professor Dominik Marx, *Lehrstuhlinhaber*, and formerly by Professor Werner Kutzelnigg) hosts several research groups including junior research groups (*Habilitanden/Nachwuchsgruppen*). All groups share common interests in "molecular systems" but taken together they also cover a substantial part of the entire spectrum of Theoretical Chemistry, see the Research / *Forschung* and the Media Gallery / *Mediathek* items on this site for details. Typically there are more than twenty scientists affiliated to Theoretical Chemistry at RUB being an international mix of physicists, chemists, and biochemists. This is supplemented by short- to mid-term visiting professors, scientists, and PhD students in the framework of collaborations or exchange programs.

The Center for Theoretical Chemistry offers a broad *and* profound program in undergraduate, graduate, and postgraduate teaching and training in modern Theoretical Chemistry and Biochemistry. PhD students are affiliated to the "Graduate School of Chemistry and Biochemistry" (GSCB) offering a rich spectrum of lectures and courses. The School runs specially tailored programs aimed at foreign PhD students covering both scientific and cultural events. In addition to having the possibility to attend the regular series of Theoretical Chemistry Colloquia (held in English) the students and postdocs will have the opportunity to be trained in complementary skills in the field of hardware and software management in a complex environment.

The Center for Theoretical Chemistry at RUB is well equipped with Computer hardware and software. This includes high-end graphics desktop PCs for each member - offices are spacious, well equipped and are shared by two or three colleagues - and a farm of servers for code development and tests supplemented by state-of-the-art graphics facilities. For applications and production runs Theoretical Chemistry operates a broad range of computational resources. These machines include several PC-based compute servers, multiprocessor alpha workstations, and altogether ten different clusters. Five of these clusters have a high speed Infiniband interconnect (up to ConnectX HCAs with DDR bandwidth) whereas the remaining clusters have at least one dedicated gigabit ethernet network. The number of two-way nodes varies from 8 to 112. Altogether, the local equipment adds up to more than 23 TeraFlop/s of computing power, nearly 7 TeraByte of RAM, and 64 TeraByte of RAID5 or RAID6 disk space. This is supplemented by the RUB Computer Center and several other parallel platforms in the state (*Ressourcenverbund NRW*) and also by grants from several National Supercomputer Centers (*Höchstleistungsrechenzentren*) in Germany. Thus, TheoChem@RUB offers a superb environment for learning, applying, and developing High-Performance Scientific Computing in Molecular Science.

Ruhr-Universität Bochum is committed to promoting the careers of women and therefore actively welcomes applications from female candidates. As an equal opportunities employer, we also encourage applications from suitably qualified disabled candidates and other groups.

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## **Postdoc and PhD Student Positions: Covalent Mechanochemistry and Molecular Nanomechanics**

**Center for Theoretical Chemistry, University of Bochum, Germany**

Applications are invited to apply for several PhD and Postdoctoral Research Fellow positions, which are available immediately or upon mutual agreement.

Candidates with a strong background in one of the following subdisciplines of theoretical chemistry and physics are most welcome: electronic structure calculations, statistical mechanics (both numerical and analytical) and/or molecular simulation. She or he will be involved in a number of challenging projects within the realms of the emerging fields "covalent mechanochemistry" and "molecular nanomechanics" developed in this group, see e.g. PRL 100 (2008) 115503, PRL 95 (2005) 096102, JACS 126 (2004) 12103, Angew. Chem. Int. Ed. 42 (2003) 2251.

Information on the techniques used and developed at CTC are accessible via [www.theochem.rub.de/go/cprev.html](http://www.theochem.rub.de/go/cprev.html). The Center for Theoretical Chemistry at RUB offers an exciting interdisciplinary research environment and excellent facilities including several high-performance parallel platforms in house, see [www.theochem.rub.de/go/jobs.html](http://www.theochem.rub.de/go/jobs.html).

Candidates should send a detailed resume including an outline of their research achievements and interests as well as contact information to obtain academic references to:

Professor Dominik Marx  
Lehrstuhl fuer Theoretische Chemie  
Ruhr-Universitaet Bochum  
44780 Bochum, Germany  
Email: [theochem@theochem.rub.de](mailto:theochem@theochem.rub.de)

There is no deadline. Consideration of candidates will begin immediately and continue until the position is filled.

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## **Group Leader and Postdoc Positions: Ab Initio Biomolecular Simulation**

**Center for Theoretical Chemistry, University of Bochum, Germany**

Applications are invited to apply for a Postdoctoral Research Fellow position, which is available immediately or upon mutual agreement. Depending on the applicant's profile there will be the opportunity for establishing an Independent Research Group and for academic qualification in the framework of Habilitation.

The ideal candidate should have significant experience in electronic calculations of complex biomolecular systems and reactions, including preferentially multiscale QM/MM--type approaches. A PhD in theoretical physics or chemistry is required, as well as research experience as a postdoc. She or he will be involved in a number of challenging projects in the realms of ab initio biomolecular simulation (see e.g. some of our recent papers: JACS Commun. 130, (2008) 2768; PNAS 104 (2007) 20725; PNAS 104 (2007) 6980; JACS 128 (2006) 13815).

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## **Postdoc and PhD Student Positions: Surface Chemistry and Heterogeneous Catalysis**

**Center for Theoretical Chemistry, University of Bochum, Germany**

Applications are invited to apply for several PhD and Postdoctoral Research Fellow positions, which are available immediately or upon mutual agreement.

The ideal candidate should have significant experience in periodic density functional calculations involving complex surfaces, interfaces and molecules. A PhD in theoretical physics or chemistry is required, as well as research experience as a postdoc. He or she will be involved in a number of challenging projects in the realms of surface chemistry, heterogeneous catalysis and nanostructured surfaces (see e.g. *Angew. Chem. Int. Ed.* 46 (2007) 4894; *PRL* 95 (2005) 096102; *Angew. Chem. Int. Ed.* 43 (2004) 6641). The project will strongly benefit from interactions within the Collaborative Research Center SFB 558 ([www.sfb558.de](http://www.sfb558.de)).

Information on the techniques used and developed at CTC are accessible via [www.theochem.rub.de/go/cprev.html](http://www.theochem.rub.de/go/cprev.html). The Center for Theoretical Chemistry at RUB offers an exciting interdisciplinary research environment and excellent facilities including several high-performance parallel platforms in house, see [www.theochem.rub.de/go/jobs.html](http://www.theochem.rub.de/go/jobs.html).

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We are constantly looking for excellent students (BSc, MSc, PhD) and postdocs. In addition, we frequently employ undergraduate students to help us maintain our computational resources with regard to both software and hardware in a complex setup.

In addition, we welcome applications for hosting Marie Curie, DAAD, Alexander von Humboldt, Emmy Noether, Heisenberg and other **fellows**. You will be member of a stimulating research group and profit from the excellent research facilities at the Ruhr-Universität Bochum!

We also help students find work experience places or summer student positions in the area of theoretical chemistry in the **chemical industry** and at the **John von Neumann Institute for Computing** (NIC) or the **Zentralinstitut für Angewandte Mathematik** (ZAM) of the research center Jülich (FZJ).

Please contact the Theoretical Chemistry secretary for more specific information. Please note, that you should contact us well in advance to avoid any complications.