Registration

To register, please visit www.mcs.uni-oldenburg.de.
The deadline for registration is **May 15, 2014**.

All participants are asked to complete a questionnaire stating their fields of interest and previous knowledge.

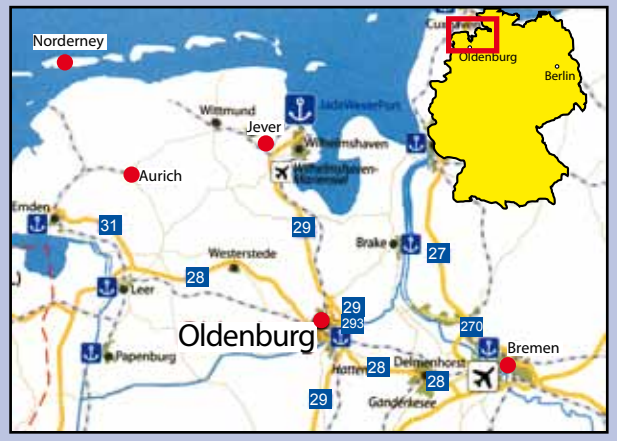
We offer a limited number of grants (including accommodation, breakfast, dinner, course material, and, for DAAD grants, travel support) for Bachelor, Master, and Diploma students. Recipients of grants only have to pay a small fee of **100 €**. For details about the application process, see www.mcs.uni-oldenburg.de. Notification about the success of the applications will be sent out until **June 1, 2014.**

We also (partially) support the option to register immediately by paying a discounted fee of 900 EUR (including accommodation in a 3-star hotel, breakfast, dinner, and course material). As a third option, you can register for a fee of 250 EUR (including dinner and course material, but with self-organized accommodation, e.g. youth hostel).

Accommodation

Room reservations (including breakfast) have been made in a 3-star hotel in the city center. The registration fee also includes dinner at the Wechloy Campus.

The dining facilities at the Wechloy Campus (same building) or at the Haarentor Campus (a 15-minute walk away) offer a variety of lunch choices.



Organization

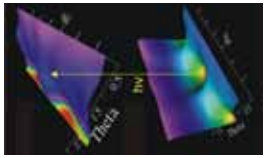
Carl von Ossietzky Universität Oldenburg
Dr. S. Harfst
Prof. Dr. A. K. Hartmann
Prof. Dr. T. Klüner

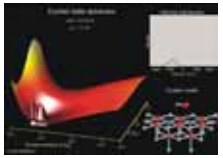
Contact

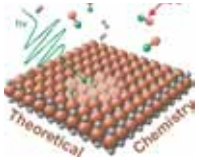
mcs@uni-oldenburg.de
Please refer to the website www.mcs.uni-oldenburg.de
for updates and more detailed information.

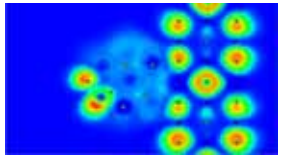
Sponsored by:

DAAD Deutscher Akademischer Austausch Dienst
German Academic Exchange Service







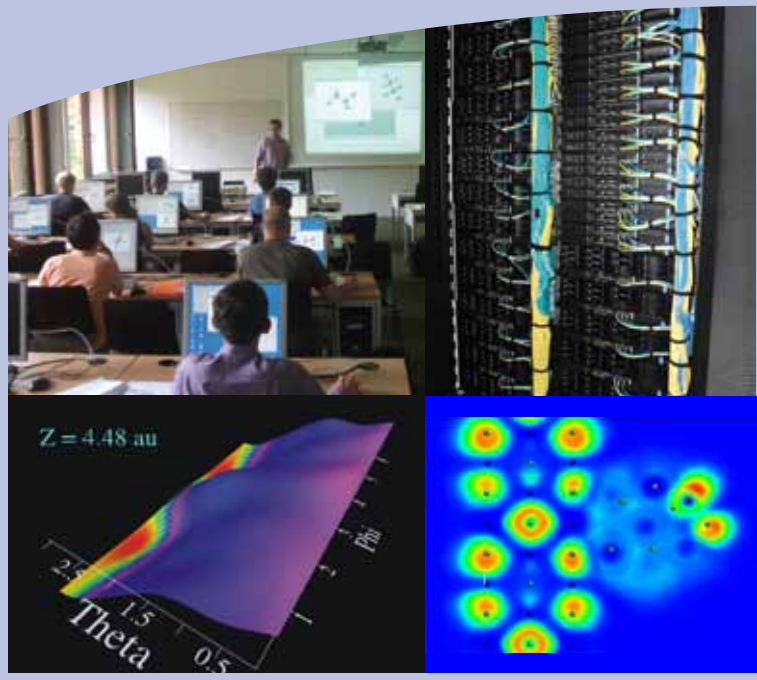


CARL VON OSSIETZKY universität OLDENBURG

Summer School

MODERN COMPUTATIONAL SCIENCE

COMPUTATIONAL QUANTUM CHEMISTRY



August 25 – September 5, 2014
University of Oldenburg, Germany

Overview

The theoretical chemistry of interfaces and surfaces is a highly topical field of research, bearing applications in fields as diverse as material science, energy research and heterogeneous catalysis. Thereby, the atomistic description of complex chemical processes routinely requires a quantum theoretical approach. It thus constitutes a huge challenge, demanding the utilisation of sophisticated and up-to-date numerical methods. Consequently, since computations on a molecular level are numerically very demanding, researchers working in the context of theoretical chemistry tradtionally belong to the key users of high performance computing (HPC) facilities.

The scope of this Summer School is twofold: in the first part it aims to deepen the understanding of the basic theoretical principles of Computational Quantum Chemistry, and in the second part it will demonstrate the application of quantum chemical methods to current problems in surface science.

In doing so, a central concern of the Summer School is to convey modern programming techniques that assure the optimal usage of computational resources. For this purpose, the Summer School will offer two intensive computer labs, focusing on code optimization and parallelisation strategies, that will utilize the local HPC cluster HERO and deepen the participants knowledge via a hands-on approach.

This Summer School addresses students from Master level onwards (including PhD students) who wish to learn more about recent developments in Computational Quantum Chemistry. Participants should have a basic knowledge of a higher programming language like C/C++ or Fortran. Further, fundamental knowledge of mathematics, quantum physics, and algorithms and data structures are beneficial.

Topics

Fundamentals: second quantization, basis sets and integrals, the Hartree-Fock method, theoretical surface science software engineering and parallelization strategies, basic numerical optimization

Theory and Applications: surface photochemistry, experimental surface science, stochastic optimization, code optimization for quantum chemistry

High Performance Computing Exercises: parallelization strategies (MPI and openMP), code optimization for non-parallel applications

External Lecturers

Georg Hager, Regionales Rechenzentrum Erlangen
Willem M. Klopper, Karlsruher Institut für Technologie
Rolf Rabenseifner, Höchstleistungsrechenzentrum Stuttgart
Volker Staemmler, Ruhr Universität Bochum

Lecturers from the University of Oldenburg

Alexander Hartmann, Computational Theoretical Physics
Martin Holthaus, Condensed Matter Theory Group
Thorsten Klüner, Theoretical Chemistry
Niklas Nilius, Scanning Probe Spectroscopy

Course Material

Each participant will receive a copy of the book *A Practical Guide to Computer Simulations* by A. K. Hartmann.

Venue

The Summer School will be held at the Wechloy Campus of the University of Oldenburg, offering a pleasant environment and plenty of nearby amenities.

Social Events

On Wednesday, August 27, participants will be invited to a barbecue.
Excursions will be organised on Wednesday afternoons and on the weekend.

Isle of Norderney

Jever Brewery

City of Bremen

wind turbine