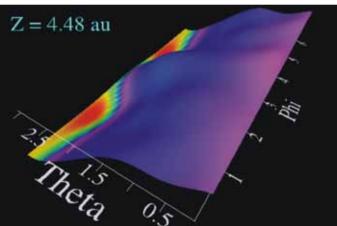


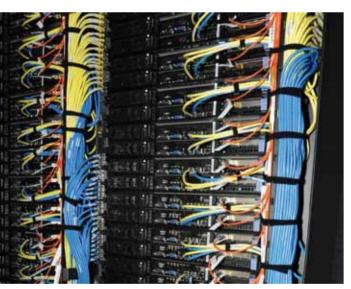
## Summer School

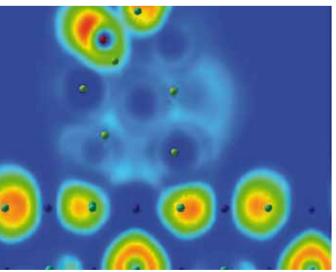
August 25 – September 5, 2014, University of Oldenburg, Germany

# MODERN COMPUTATIONAL SCIENCE COMPUTATIONAL QUANTUM CHEMISTRY











#### **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

for advanced (including PhD) students
in the Natural Sciences, Mathematics, Informatics, and Engineering

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