MAPEX Bremen
Material. Process. Excellence.

03
10-2016

INSTRUMENT DATABASE
High Performance Computing Cluster QM3

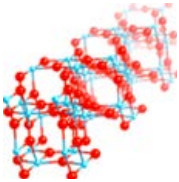
Universität Bremen

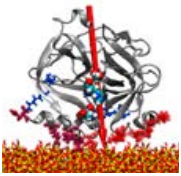
BREMEN CENTER FOR COMPUTATIONAL MATERIALS SCIENCE (BCCMS)

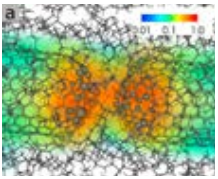
BCCMS Bremen Center for Computational Materials Science

The Bremen Center for Computational Materials Science – BCCMS was founded in 2006 as an interdisciplinary research center of the science and engineering faculties at the University of Bremen.

The available materials and process simulation expertise ranges from many-body electron theory (Prof. Tim Wehling), quantum mechanical materials modelling (Prof. Thomas Frauenheim), atomistic and mesoscopic coarse-grained (CG) modelling (Prof. Lucio Colombi Ciacchi) up to microstructure evolution modelling (Prof. Vasily Ploshikhin). The aim is to merge the multi-scale expertise of different fields in computational materials science, life science, and engineering in order to address urging questions related to future materials development in renewable energy, safe environment, transportation, and health. The new computing cluster will be of special benefit for the twelve PhD students within the recently established Research Training Group 2247 "Quantum Mechanical Materials Modelling QM³" that is coordinated by the two MAPEX members Thomas Frauenheim and Tim Wehling.







From left to right:

1) Atomic structure of Fe-hydrogen complex adsorbed on a Pt(111) surface.

2) Fundamental electronic properties of TiO_2: bulk, surfaces, interfaces, nanostructures.

3) Protein adsorption on solid surfaces studied with quantum mechanical and classical Molecular Dynamics.

4) Prediction of electrical properties of carbon-nanotube- reinforced polymers.

Due to a number of significant advances in first-principles quantum-mechanical, classical atomistic, coarse graining, and finite element calculations over the past decade, coupled with the highly improved efficiency of software and computer architectures, it is only now becoming possible to investigate materials at a very high level of theory and under operational and loading conditions, fully taking into account atomistic and electronic details with reliable experimental accuracy.

|| HIGH PERFORMANCE COMPUTING CLUSTER QM3

01 || General Information

Keywords: quantum mechanics, molecular transport, electronic conductivity, DFT, materials properties, nanoscale simulations, electronic correlation and transport, low-dimensional systems, molecules at surfaces

Categories

- Computing

Main application: theoretical physics, chemistry and materials science on atomistic scale including electronic degrees of freedom.

Year of Fabrication: 2016

Manufacturer: Megware Computer GmbH

02 || Specifications

- 109 compute nodes
- 20xE5-2660v3 cores per node, 2180 total cores
- 128 GByte RAM per node
- Intel OmniPath high-performance interconnect
- BeeGFS scratch storage with 175 TByte of space
- Operating System CentOS 7

03 || Contact

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