The foundation of the BCCMS and computational approaches to advanced materials design

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The Bremen Center for Computational Materials Science – BCCMS was founded in 2006 as interdisciplinary institute of the science and engineering faculties at the University of Bremen. The BCCMS now consists of four groups, the Foundation Chair ``Computational Materials Science - CMS´´, the Endowed Conrad Naber Chair ``Hybrid Materials Interfaces – HMI´´, the Endowed Airbus Chair ``Multiscale Materials Modelling & Engineering – MMME´´ and the new Theoretical Physics group ``Electronic structure and correlated nanosystems´´.

By using state-of-the-art multiscale methods ranging from quantum and atomistic simulations over coarse-graining approaches to micro- and macroscopic continuum theory, the applications particularly focus on structural design of complex materials in order to develop novel functional materials and devices in close cooperation with experimental and industrial partners.

The CMS-Group at the Faculty of Physics has strong record in electronic structure methods ranging from ab initio quantum theory towards approximate density functional schemes with the major interest to perform chemically reactive studies on nanomaterials, biosystems and complex surfaces/interfaces. As major label of the group, the DFTB-method and the related DFTB+-Software recently is distributed for academic research to the world wide user community, see http://www.dftb.org.

Currently , the BCCMS has been expanded with two additional Endowed Faculty Chairs. The ``Hybrid Materials Interfaces - HMI´´ Group at the Faculty of Production Engineering is chaired by Lucio Colombi Ciacchi since October 2008 . The focus of its research lies on the atomic-level studies of interfaces between technological materials and biological macromolecules, with applications in the fields of biomedical implants, biosensors, pharmaceutical packaging, biocompatible adhesives, and others.

End of 2009, the Endowed Airbus Chair ``Integrative Simulation & Engineering of Materials and Processes – ISEMP´´, has been established at the Faculty of Physics. This profile is complementing the computational activities in top-down approach from the macro- and microstructure scale modeling.

Most recently, Tim Wehling has joined the BCCMS as Junior Professor for ``Electronic Structure and Correlated Nanosystems – ECN´´. His research group is contributing computational expertise in many-body physics and applications to solid state and nanomaterials showing strong electron correlations. Research interests include the electronic properties of graphene-based systems, novel layered materials, and magnetic nanostructures on surfaces.

The major research activities of the BCCMS will be shortly summarized and results including multiscale method developments and applications to hybrid- and biomaterials interface design will be discussed.