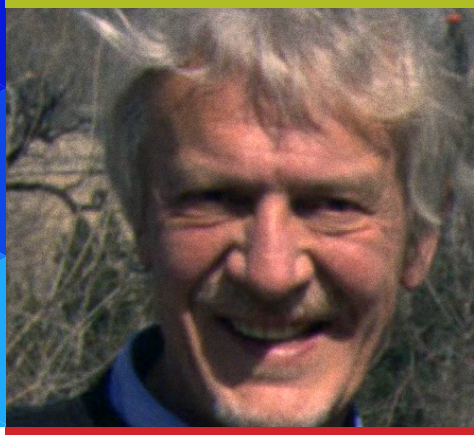
Skoltech
Skolkovo Institute of Science and Technology

Computational Materials Science Seminar

DFTB+ - AN APPROXIMATE DFT METHOD:

Applications to computational nanomaterials

April 18th
16:00-17:00
room 403

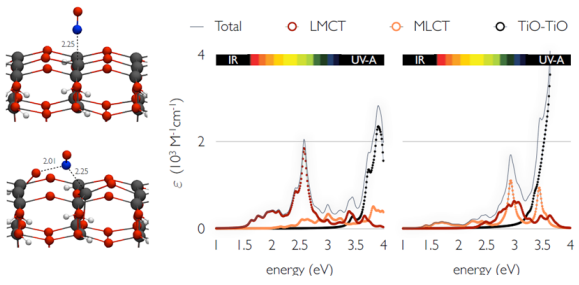


Abstract:

The new release of DFTB+ as a density-functional (DFT)-based approach, combining DFT-accuracy and Tight-Binding (TB) efficiency, is reported; http//:www.dftb.org. Methodological details and recent extensions to improve reliability and accuracy will be described briefly. Advanced functions include spin degrees of freedom, time dependent methods for excited state dynamics, and multi-scale QM/MM/Continuum-techniques to treat reactive processes in nanostructures under environmental conditions. Additionally, the combination with non-equilibrium Green´s functions allows to simulate quantum transport in nanoscale devices and on the molecular scale.

As one latest application chemical vapor deposition (CVD) graphene growth on Cu(111) has been modeled with DFTB molecular dynamics simulations. These simulations demonstrate at the atomic level how high-quality graphene forms on Cu-(111) surfaces. In contrast to other popular catalysts, such as nickel and iron, copper is in a surface molten state throughout the graphene growth at CVD-relevant temperatures supporting 5- and 7-membered ring defects to heal over time.

Very recently the time-dependent density functional based tight-binding (TD-DFTB) approach is generalized going beyond the Mulliken approach. An additional on-site correction leads to marked qualitative and quantitative improvements over the original method. Especially, the known failure of TD-DFTB for the description of $\sigma \rightarrow \pi^*$ and $n \rightarrow \pi^*$ excitations is overcome. Benchmark calculations on a large set of organic molecules also indicate a better description of triplet states. As application we report on excited-state theoretical simulations and experimental studies to investigate the degradation of nitric oxide and acetaldehyde on TiO2 under VIS and UV irradiation revealing charge transfer complexes on TiO2 as new source for visible light activity. Figure below: NO adsorption on anatase and absorption spectra.



Looking forward to seeing you!

Speaker

Thomas Frauenheim
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BIO: Since the mid-90th Thomas Frauenheim has pioneered the development of the density-functional based tight-binding method (DFTB) which combines the high efficiency of semi-empirical methods with the accuracy of ab initio density-functional theory (DFT). The new implementation of the method, DFTB+ http://www.dftb-plus.info/overview/. is the most distributed and used software of it´s type, worldwide. The functionality includes open shell capabilities (Christof Koehler), non-collinear magnetism, LDA+U, GW, TD-DFTB in linear response and in the time-domain, the non-equilibrium Green´s-Function implementation for charge transport and various QM/MM-coupling schemes to classical force fields.
As director of the German CECAM-Node ***Multi-scale modelling from 1-st principles*** since 2009 he has initiated noumerous International CECAM-Workshops and hands-on-tutorials on atomistic simulations bringing together world leading experts and young researchers from computational solid state and materials physics, theoretical chemistry and molecular biology, promoting a new quality of scientific networking and exchange of knowledge and software developments http://www.bccms.uni-bremen.de/events/.