DFTB+ - An approximate DFT method: Applications to computational nanomaterials

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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 will be described briefly. Advanced functions include spin degrees of freedom, time dependent methods for excited state dynamics, efficient Order-N algorithms 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 address quantum transport in nanostructures and on the molecular scale.

Structure formation under technological relevant conditions is controlled by Molecular-Dynamics Simulated Annealing in ground and excited states. Successful applications are shown to cover a broad spectrum of problems, ranging from semiconductor nanostructures through amorphous materials to hybrid-interface design. Some detailed examples include studies of optical properties of functionalized semiconductor quantum dots and inelastic electron tunneling spectra in transport through single molecule junctions.

Approaching new frontiers in materials science the DFTB-method is generalized and improved to cover also weak interactions and extended to QM/MM/Continuum-coupling for applications to functional biosystems. Recent work include the proton blocking in aquaporine channels and the spectral tuning in retinal protein photocycles. The QM/MM concepts, originally developed for biosystem-simulations are generalized to the study of bulk problems and surface adsorption.