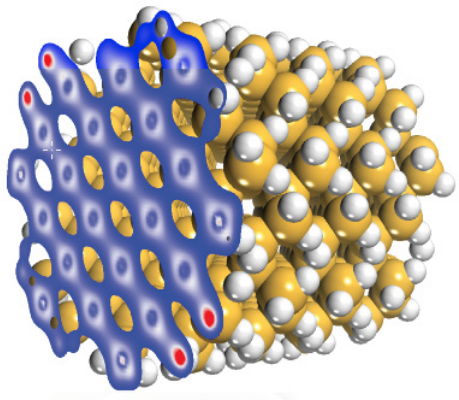
BIOVIA MATERIALS STUDIO DFTB+

DATASHEET

BIOVIA Materials Studio DFTB+ is an improved implementation of the Density Functional based Tight Binding (DFTB) quantum simulation method for the study of electronic properties of materials. Combining near quantum mechanical accuracy with solution speeds approaching those of classical atomistic methods, Materials Studio DFTB+ offers unique capabilities to study and understand systems containing hundreds of atoms. Problems that took more time or compute power than most researchers have available, such as defects in semi-conductors, and interactions between organic and inorganic surfaces, are now practical to study using Materials Studio DFTB+. These types of problems are common throughout several industry sectors including catalysis, electronics, and chemicals.

WHAT DOES BIOVIA MATERIALS STUDIO DFTB+ DO?

Materials Studio DFTB+ enables the optimization and study of dynamical properties of materials with quantum mechanics accuracy but in significantly less time. Structures can be optimized and molecular dynamics used to study the temporal evolution of the structure. Properties such as band structure, and atomic orbitals and Fermi surfaces can be calculated and visualized, giving a deep understanding of the electronic structure of materials. Population analysis and electron density can be used to visualize charge distribution. Materials Studio DFTB+ uses libraries of parameters called Slater-Koster files to encapsulate the interactions between the elements in the material. If the elements are not parameterized, Materials Studio DFTB+ includes a specific parameterization task to develop new parameter sets, enabling extension to new systems.



KEY USES OF MATERIALS STUDIO DFTB+

Semiconductors

The ability to model systems containing thousands of atoms enables researchers using semi-conductors to study the effect of defects on their systems.

Surface adsorbed monolayers

Capturing both the interactions at the surface between a monolayer and surface and the bulk of the monolayer requires tools that can give an accurate electronic description but still be applied to a large number of atoms. Materials Studio DFTB+ satisfies both of these requirements, making it applicable to a wide range of calculations where either quantum mechanics approaches are too expensive, or forcefield descriptions do not capture the level of detail.

Growth of structures on surfaces

Studying growth of inorganic crystals such as boron nitride on diamond surfaces requires the ability to model bond formation and breaking and do this on a large scale. Materials Studio DFTB+ provides the accurate electronic structure calculation and couples this with large system sizes, enabling the study of realistic growth models.

THE MATERIALS STUDIO ADVANTAGE

Materials Studio DFTB+ is operated from within the Materials Studio® environment. Materials Studio provides an integrated user interface that is easy to use and quick to learn. Materials Studio Visualizer, the core Materials Studio product, offers a wide range of model building and visualization tools that allow you to rapidly construct models of the system of interest, perform Materials Studio DFTB+ calculations, and analyse the results. Integration in Materials Studio means that generating new parameters is a single task which seamlessly utilizes the Materials Studio DMol³ density functional theory module.

A flexible client-server architecture means that calculations can be run on servers located elsewhere on your network. Results are returned to your PC, where they may be displayed and analyzed. You can easily produce high quality graphics of structures, including electron density maps. These structures, graphs, and other data such as video clips, produced from Materials Studio DFTB+ output, can be instantly exchanged with other PC applications.

HOW DOES MATERIALS STUDIO DFTB+ WORK?

DFTB is based on Density Functional Theory (DFT) but uses empirical approximations to improve the performance whilst maintaining accuracy. The main approximation in the tightbinding approach is the replacement of the exact many-body Hamiltonian in DFT with a parameterized Hamiltonian matrix. In the DFTB description pseudo atomic wave functions, written in terms of Slater-type orbitals and spherical harmonics, are used to model the electron density. The orbital basis is fitted to against DFT theory and then used to calculate the Hamiltonian and overlap matrix elements. The DFTB approach uses approximations to expand the total energy of the DFT representation to the second order in charge density and spin density fluctuations.

The matrix elements do not fully describe the total energy of the system, the remaining part of the total energy is included as a short-range repulsive term which can be described in terms of pair wise potentials between atoms. The pair wise potentials are acquired through a fitting process.

For systems where the balance of charges between pairs of atoms is very small, Materials Studio DFTB+ also uses self consistent charge (SCC-DFTB) to improve the description of the bond. In order to simplify the calculations, the SCC calculation is performed on Mulliken charges rather than the potential and charge density.

Besides the usual electronic and short-range repulsive terms, the final approximate Kohn-Sham energy additionally includes a Coulomb interaction between charge fluctuations. At large distances this accounts for long-range electrostatic forces between two point charges and approximately includes selfinteraction contributions of a given atom if the charges are located at one and the same atom. Due to the SCC extension, DFTB can be successfully applied to problems where deficiencies in the non-SCC standard TB approach become obvious.

FEATURES AND CAPABILITIES

Calculation tasks

- Single point energies
- Geometry optimization including options to optimize cell and perform rigid body optimization
- Molecular dynamics using NVE, NVT, NPH and NPT ensembles
- Parameterization task for creating new Slater-Koster parameter sets fitting to LDA/PWC, GGA/PW91 or GGA/PBE functionals
- All tasks work on non-periodic and periodic systems
- Include van der Waals dispersion corrections
- Fermi (Non-metallic systems) and Methfessel-Paxton (Metallic systems)
- Restricted and un-restricted calculations
- Accelerated SCF convergence with smearing

Parameters

- CH – parameters for hydrocarbons
- CHNO – parameters for molecules containing carbon, hydrogen, nitrogen and oxygen
- SiGeH – parameters for semi-conductors containing silicon, germanium and hydrogen
- SiBand - (Si-O-H) - parameters for electronic structure for Si, SiO2 and their interfaces
- MagSil - (Mg)-(Mg,Si,H,O) – parameters for electronic and mechanical properties of chrysotile nanotubes
- Range of specialist parameter sets described at **http://www.dftb.org/**

Properties

- Mechanical Properties
- Full density of states
- Full band structure
- Electron density visualization
- Fermi surface visualization
- Orbital energies and visualization
- Population analysis

To learn more about Materials Studio, go to **3dsbiovia.com**/materials-studio

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