CASTEP
DATASHEET

BIOVIA Materials Studio CASTEP is an ab initio quantum mechanical program employing density functional theory (DFT) to simulate the properties of solids, interfaces, and surfaces for a wide range of materials classes such as ceramics, semiconductors, and metals. First principle calculations allow researchers to investigate the nature and origin of the electronic, optical, and structural properties of a system without the need for any experimental input. BIOVIA Materials Studio CASTEP is thus well suited to research problems in solid state physics, materials science, chemistry, and chemical engineering where empirical models are lacking and experimental data may be sparse. In these areas, researchers can employ computer simulations to perform virtual experiments, leading to tremendous savings in costly experiments and shorter developmental cycles.

WHAT DOES BIOVIA MATERIALS STUDIO CASTEP DO?

Researchers in chemistry and materials science may be tasked with a number of challenging goals like the development of new compounds, such as a stronger light-weight alloy or a semiconductor that will make a faster computer chip; or they may need to improve a manufacturing process that uses atomic layer deposition; or they may be faced with simply understanding and describing fundamental processes, explaining why one particular material is better than another. Modeling can address all of these challenges, provided that the method is fast, accurate, and works at the atomic scale. BIOVIA Materials Studio CASTEP is just such a method.

Originally developed in the Theory of Condensed Matter Group at Cambridge University, UK, BIOVIA Materials Studio CASTEP uses quantum mechanical calculations to study problems in chemicals and materials research. A large number of academic and commercial partners assures that the program incorporates the latest technologies and has been well-validated for the types of problems faced by research scientists in the fields mentioned above.

BIOVIA Materials Studio CASTEP is able to predict the structure of a material as well as many essential properties. In particular, it can predict electronic properties such as band gaps and Schottky barriers; optical properties such as phonon dispersion curves, polarizability and dielectric constants; or physical properties such as elastic constants. Put these all together to get a tool for the rapid and accurate design of new materials in silico.

Key features include a transition state search algorithm that greatly facilitates determination of reaction profiles and energy barriers, essential to an understanding of kinetics. The full 6x6 tensor of the elastic constants can be predicted for a periodic structure of any symmetry. Recent advances in the ability to compute phonon frequencies makes it possible to predict thermodynamic properties such as free energy and heat capacity for any material. Moreover, the ability to make thermodynamic predictions of solid-state systems enables the simulation of many condensed matter properties such as the phase stability of structural modifications.

Based on total energy pseudopotential methods, BIOVIA Materials Studio CASTEP requires as input only the number and type of atoms in a system and predicts properties such as lattice constants, molecular geometry, elastic constants, bandstructures, density-of-states, charge densities and wave functions, and optical properties. The pseudopotential plane-wave technology underlying BIOVIA Materials Studio CASTEP is well validated, with hundreds of scientific publications written each year demonstrating new applications of the code. Efficient parallel versions of the code are also available for large systems involving hundreds of atoms.

BIOVIA Materials Studio CASTEP has been applied to a wide range of research problems such as surface chemistry, physi- and chemisorption, heterogeneous catalysis, defects in semiconductors, grain boundaries, stacking faults, nanotechnology, molecular crystals, polymorphic studies, diffusion mechanisms, and molecular dynamics of liquids.

THE BIOVIA MATERIALS STUDIO ADVANTAGE

BIOVIA Materials Studio CASTEP is part of the BIOVIA Materials Studio® software environment. BIOVIA Materials Studio provides a user-friendly interface, complying with Windows® standards. Materials Visualizer, the core BIOVIA Materials Studio product, offers a wide range of model building and visualization tools that allow you to construct rapidly models of the systems of interest, easily select the BIOVIA Materials Studio CASTEP module, and run an advanced quantum mechanical calculation. The simple user interface together with BIOVIA's training programs ensure that even new users will be able to use the program with confidence.
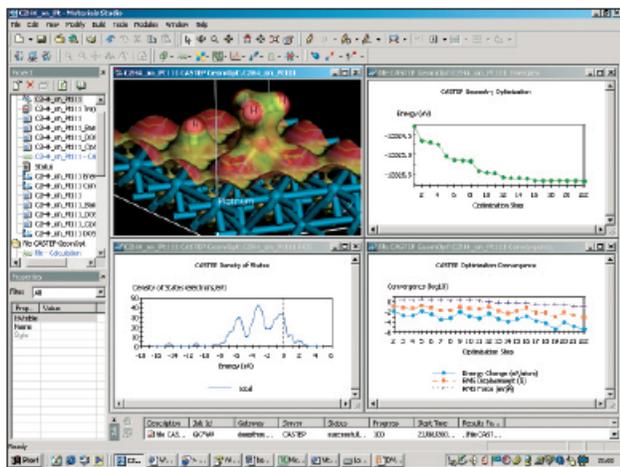
C_2H_4 absorption on a Pt (111) surface showing the electrostatic potentialprojected on the electronic density isosurface. Density of states, energy evolution, and energy convergence graphs are also shown.

A flexible client-server architecture means that calculations can be run on servers located anywhere on your network. Results are returned to your PC, where they may be displayed and analyzed. You can easily produce high-quality graphics of geometric structures, molecular orbitals, electrostatic potentials, or charge densities. Structures, graphs, and other data such as video clips produced from BIOVIA Materials Studio CASTEP output can be instantly exchanged with other PC applications, assisting you when sharing them with colleagues or when analyzing your results using spreadsheets and other packages.

HOW DOES BIOVIA MATERIALS STUDIO CASTEP WORK?

BIOVIA Materials Studio CASTEP1-3 uses a total energy plane-wave pseudopotential method. In the mathematical model of the material, BIOVIA Materials Studio CASTEP replaces core electrons with eff ective potentials acting only on the valence electrons in the system. Electronic wavefunctions are expanded through a plane-wave basis set, and exchange and correlation effects can be included within either the local density (LDA) or generalized gradient (GGA) approximations. Combining the use of pseudopotentials and plane wave basis sets enables extremely efficient geometry optimizations of molecules, solids, surfaces, and interfaces. The primary reason that BIOVIA Materials Studio CASTEP has become so powerful is that the numerical methods used to solve the underlying quantum mechanical calculations are both computationally effi cient and extremely accurate.

BIOVIA Materials Studio CASTEP is capable of computing many electronic and optical properties using density functional perturbation theory (DFPT), also known as the linear response method. This approach makes possible a wider variety of properties than are possible using the so-called fi nite diff erence approaches, which require repeated computations on a series systems. Using DFPT, BIOVIA Materials Studio CASTEP can predict a number of significant observables including the phonon density of states, phonon dispersion, optical polarizability, IR spectra, and dielectric functions.

FEATURES AND CAPABILITIES

Calculation Tasks
- Total energies, forces, and stresses
- Many exchange-correlation functionals including B3LYP
- Geometry optimizations (including unit cell parameters)
- Molecular dynamics using NVE, NVT, NPH, and NPT ensembles
- Transition state search based on the linear and quadratic synchronous transit methodology (LST/QST)
- Elastic constants
- Phonon frequencies using linear response or finite displacements

General Capabilities
- Choice of local, gradient-corrected, and nonlocal functionals for approximating exchange and correlation effects
- Nonlocal functional include screened-exchange, HF, B3LYP and PBE0
- LDA+U method for strongly correlated systems, including magnetic systems
- Semi-empirical dispersion correction schemes
- Ultra soft and norm-conserving pseudopotentials for the entire periodic table

Job Control Options
- Choice of parallelization strategy to optimize computational performance
- Choose number of CPU's
- Specify server machine
- Monitor output and status reports including text or graphs of energy and gradient during geometry optimization
- Live updates of the model geometry and job status
- Halt jobs on remote server via the Materials Visualizer

Properties
- Band structures
- Core-level spectra[8] like EELS, ELNES or XES
- Dielectric function polarizability, refl ectivity
- Electron work function
- IR spectra[8]
- Mulliken population analysis for atoms and bonds
- Optical properties: frequency dependent
- Phonon dispersion
- Raman spectra[8]
- Refractive index, UV spectra[8]
- Static elastic constants
- Thermodynamic properties in quasiharmonic approximations (free energy, enthalpy, entropy, heat capacity, Debye temperature)
- Total and projected phonon density of states

Graphical Displays with BIOVIA Materials Studio Visualizer

- 3-D contours and 2-D slices
- Charge, spin, and deformation densities
- Fermi surface
- Overlay multiple plots and color surfaces by property maps
- Simulated scanning tunneling microscopy (STM) images

Miscellaneous Options

- Real or reciprocal space pseudopotential representation
- Full use of space-group symmetry
- Multiple options for accelerating SCF convergence: DIIS, density mixing, smearing.

To learn more about BIOVIA Materials Studio, go to accelrys.com/materials-studio

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