BIOVIA MATERIALS STUDIO FORCITE

DATASHEET

BIOVIA Materials Studio Forcite is an advanced classical molecular mechanics tool, that allows fast energy calculations and reliable geometry optimization of molecules and periodic systems. For crystal structures, geometry optimization with BIOVIA Materials Studio Forcite retains the crystal symmetry. BIOVIA Materials Studio Forcite provides the user with great flexibility, offering a range of forcefields and charging methods. Since BIOVIA Materials Studio Forcite runs interactively in BIOVIA Materials Studio on any client PC, it offers an ideal solution to the everyday requirement of the modeler to generate optimized models and compare their energies.

WHAT DOES BIOVIA MATERIALS STUDIO FORCITE DO?

BIOVIA Materials Studio Forcite calculates single point energies and performs geometry optimization, i.e. energy minimization, of molecules and periodic systems. For periodic systems, BIOVIA Materials Studio Forcite allows the optimization of the cell parameters simultaneously with the molecular coordinates. In addition, an external hydrostatic pressure may be applied.

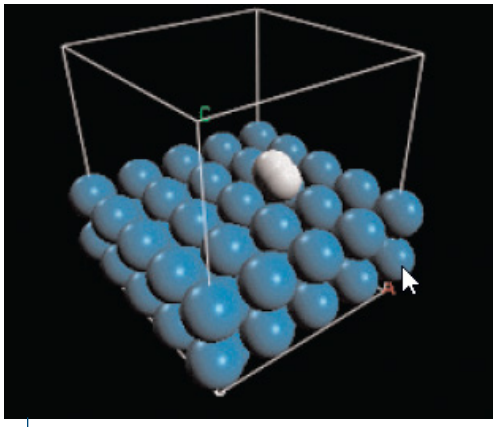

Figure 1: Hydrogen interaction with a tungsten surface. Geometry optimization with BIOVIA Materials Studio Forcite calculates the physisorption of the hydrogen molecule, which can be used as a starting structure for chemisorption simulations with BIOVIA Materials Studio DMol³ or BIOVIA Materials Studio CASTEP.

During a geometry optimization of a crystal structure, BIOVIA Materials Studio Forcite preserves the symmetry defined by the space group, and the crystal structure is optimized either with respect to all structural degrees of freedom or applying rigid body constraints where the relative distances between a group of atoms are fixed.

Since BIOVIA Materials Studio Forcite is a molecular mechanics tool, its calculations draw upon forcefields, and associated parameters settings. BIOVIA Materials Studio Forcite is designed to work with a wide range of forcefields, and give easy and flexible access to the associated parameter options.

Currently, BIOVIA Materials Studio Compass, Dreiding, Universal Force Field, CVFF, and PCFF are supported, providing the opportunity to handle any chemical system.

APPLYING BIOVIA MATERIALS STUDIO FORCITE

BIOVIA Materials Studio Forcite is operated from within the BIOVIA Materials Studio® software environment. BIOVIA Materials Studio provides a user interface that is easy-to-use and quick to learn, complying with Windows® standards.

BIOVIA Materials Studio Visualizer, the core BIOVIA Materials Studio product, runs under Windows 2000 or XP. It offers a wide range of model building and visualization tools. You can rapidly construct models of the systems that interest you, select BIOVIA Materials Studio Forcite with a single mouse click, and then run an advanced simulation.

Structures, graphs, and other data can be instantly exchanged with other PC applications, helping you to share them with colleagues and analyze them using spreadsheet and other packages.

To use the BIOVIA Materials Studio Forcite program, you begin with a molecular or periodic structure of the system you want to study. This can be constructed from the molecular structure of the component(s) by means of the Amorphous Cell module or using the Crystal Builder component of the Materials Studio interface.

You then choose a calculation task, either Energy or Geometry Optimization, desired quality level for the task, and a forcefield. Clicking on Run will submit a job to your selected server machine, using MS Modeling's advanced client-server architecture. BIOVIA Materials Studio Forcite updates the active structure document, and reports the results in text and chart documents. BIOVIA Materials Studio Forcite brings an advanced molecular mechanics tool to your desktop.

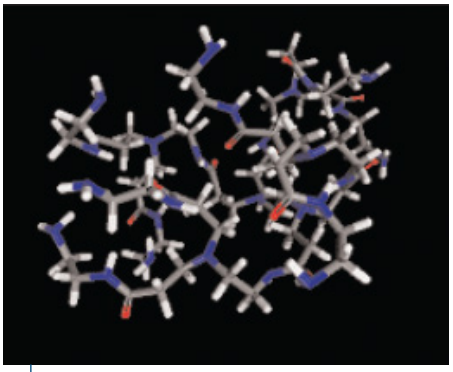

Figure 2: Geometry optimization with symmetry constraints can be carried out on crystal structures using BIOVIA Materials Studio Forcite. Structure shown is that of urea.

FEATURES

- Energy calculation of molecules, periodic, and crystalline structures
- Geometry optimization of molecules, periodic systems, and crystalline structures observing crystal symmetry
- Support of BIOVIA Materials Studio Compass, Dreiding, Universal Force Field, CVFF, and PCFF
- Charges may be calculated using the Charge Equilibration or Gasteiger methods
- Choice of Geometry Optimization algorithms: Steepest descent, Quasi-Newton, Conjugate Gradient, ABNR, or the Smart algorithm
- Optional cell optimization for periodic systems: all or a limited set of cell parameters can be optimized
- External stress may be applied to periodic models
- Calculation parameters can be set easily via various quality levels, or customized individually by the user
- Graphical output of convergence parameters, energy, cell parameters, and density where appropriate.

HOW DOES BIOVIA MATERIALS STUDIO FORCITE WORK?

BIOVIA Materials Studio Forcite draws upon an energy server, which has been designed by Accelrys to meet the demands of fast, reliable and comple energy calculations. In particular, the energy server handles constraint minimizations, which allow the geometry optimization calculation in BIOVIA Materials Studio Forcite to be performed under the constraint of crystal symmetry.

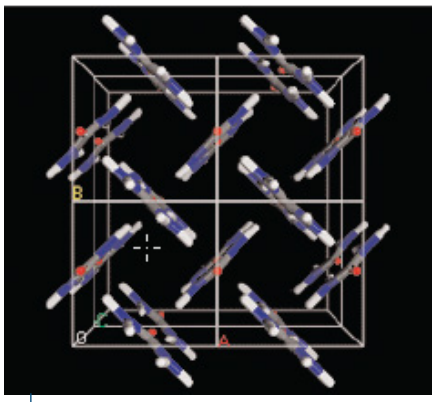

Figure 3: Geometry optimization with symmetry constraints can be carried out on crystal structures using BIOVIA Materials Studio Forcite. Structure shown is that of urea.

BIOVIA Materials Studio Forcite energy calculations can use either Atom based or, in the case of periodic systems, Group-based or Ewald summation schemes. It can access QEq and Gasteiger charging schemes to determine atomic charges.

For Geometry optimization calculations BIOVIA Materials Studio Forcite offers a choice of algorithms: Steepest descent, Quasi-Newton, Conjugate Gradient, ABNR, or the Smart algorithm, which is a cascade of the Steepest Descent,ABNR, and Quasi-Newton methods.

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

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