

FORCITE

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 Forcite retains the crystal symmetry. Forcite provides the user with great flexibility, offering a range of forcefields and charging methods. Since Forcite runs interactively in 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 FORCITE DO?

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

During a geometry optimization of a crystal structure, 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 Forcite is a molecular mechanics tool, its calculations draw upon forcefields, and associated parameters settings. Forcite is designed to work with a wide range of forcefields, and give easy and flexible access to the associated parameter options.

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

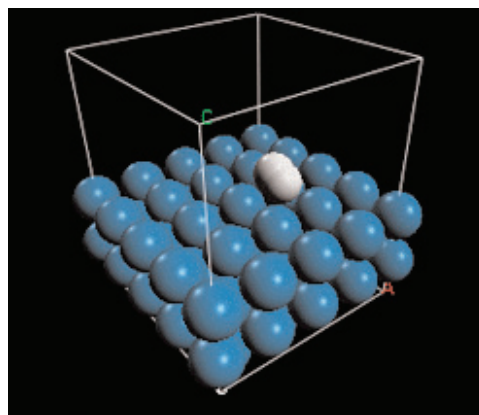


Figure 1: Hydrogen interaction with a tungsten surface. Geometry optimization with Forcite calculates the physisorption of the hydrogen molecule, which can be used as a starting structure for chemisorption simulations with DMol³ or CASTEP.

APPLYING FORCITE

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

Materials Visualizer, the core 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 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 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. Forcite updates the active structure document, and reports the results in text and chart documents. Forcite brings an advanced molecular mechanics tool to your desktop.

FEATURES

- Energy calculation of molecules, periodic, and crystalline structures
- Geometry optimization of molecules, periodic systems, and crystalline structures observing crystal symmetry
- Support of 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

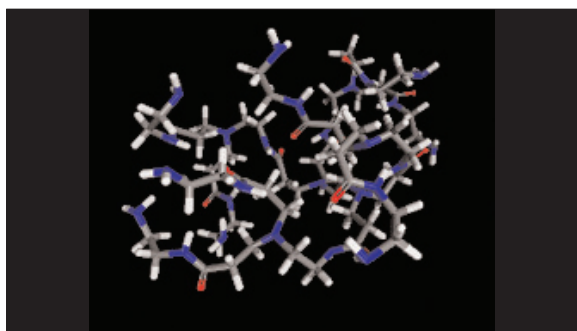


Figure 2: Geometry optimization with symmetry constraints can be carried out on crystal structures using Forcite. Structure shown is that of urea.

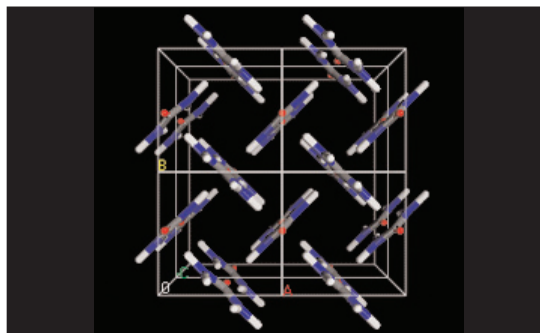


Figure 3: Geometry optimization with symmetry constraints can be carried out on crystal structures using Forcite. Structure shown is that of urea.

- 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 FORCITE WORK?

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

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 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 Materials Studio, go to accelrys.com/materials-studio