accelrys®

Materials Studio

An advanced classical molecular mechanics tool

Allows fast energy calculations and reliable geometry optimization of molecules and periodic systems

Offers a range of forcefields and charging methods

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 requirements of modelers who need 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.

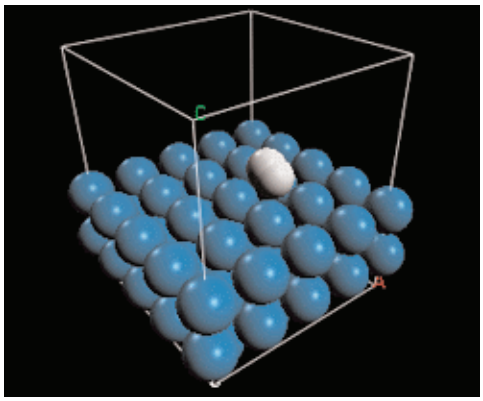
During a geometry optimization of a crystal structure, Forcite preserves the symmetry defined by the space group; the crystal structure is optimized either with respect to all structural degrees of freedom or by applying rigid body constraints where the relative distances between a group of atoms are fixed. Since Forcite is a molecular mechanics tool, its calculations draw upon forcefields and associated parameter 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, CVFF, and PCFF forcefields are supported, providing the opportunity to handle any chemical system.

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 because it complies 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



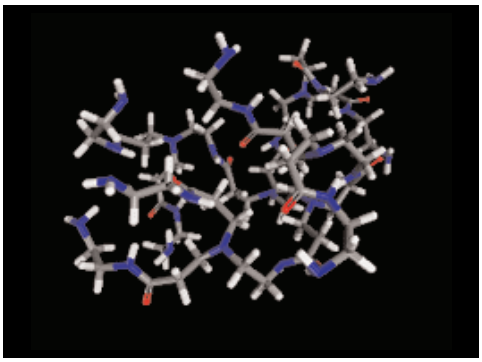
Hydrogen interaction with a tungsten surface. Geometry optimization with Forcite calculates the physisorption of the hydrogen molecule, which can be used as a starting structure for chemisorption simulations with DMol³ or CASTEP.

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 spreadsheets and other packages.

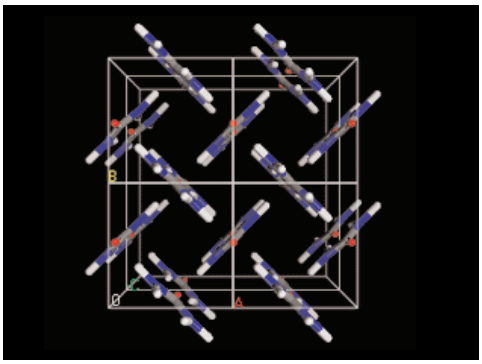
To use the Forcite program, you begin with a molecular or periodic structure of the system you want to study. This can be constructed from the molecular structure of the component(s) by means of the Amorphous Cell module or by using the Crystal Builder component of the Materials Studio interface. You then choose a calculation task (either Energy or Geometry Optimization), the desired quality level for the task, and a forcefield. Clicking on Run will submit a job to your selected server machine, using Materials Studio'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.

accelrys®

Materials Studio



Forcite provides reliable geometry optimisation of complex structures, such as the polyamidoamine (PAMAM) dendrimer



Geometry optimization with symmetry constraints can be carried out on crystal structures using 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 COMPASS, Dreiding, Universal, CVFF, and PCFF forcefields
- 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
- Rigid body optimization
- Non-bond calculations treated using atom-based, group-based, or Ewald summations
- 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
- Control by MaterialsScript API of all tasks and analysis tools in Forcite

Forcite - Analysis

- Graphical animation of dynamics run
- Breakdown of system energy during run
- Plot and analyze temperature, pressure, volume, stress, and cell parameters
- Plot and analyze distances, angles and torsions
- Plot and analyze concentration profiles in any direction
- Calculate radial distribution function and structure factor
- Calculate mean squared displacement
- Calculate dipole autocorrelation function and power spectrum
- Calculate fluctuation properties, such as isometric heat capacity
- Calculate radius of gyration
- Calculate rotational time correlation function
- Calculate X-ray and neutron scattering data
- Calculate space-time correlation function
- Calculate spatial orientation correlation function
- Calculate stress-autocorrelation function and shear viscosity
- Calculate velocity autocorrelation function
- View the trajectory data in a study table
- Plot trajectory data directly from the study table
- Sort by any property, for example sort by energy to find the lowest energy conformations
- Analyze Discover .his or .arc trajectory files

accelrys®

Accelrys Corporate Headquarters
10188 Telesis Court, Suite 100
San Diego, CA 92121–4779, USA
Tel: +1 858 799 5000

Accelrys European Headquarters
334 Cambridge Science Park
Cambridge, CB4 OWN, UK
Tel: +44 1223 228500

Accelrys Asia Headquarters
Nishi-shimbashi TS Bldg 11F
Nishi-shimbashi 3–3–1, Minato-ku,
Tokyo, 105–0003, Japan
Tel: +81 3 3578 3861

0308