BIOVIA MATERIALS STUDIO FORCITE PLUS

DATASHEET

BIOVIA Materials Studio Forcite Plus is an advanced classical mechanics tool that allows energy calculations, geometry optimizations, and dynamics simulations. It performs all of these tasks on a wide variety of structures, from simple molecules to 2D surfaces and 3D periodic structures, such as crystals. A comprehensive suite of analysis tools allows modelers to analyze a range of properties, from density variations to diffusion and solubility parameters.

WHAT DOES BIOVIA MATERIALS STUDIO FORCITE PLUS DO?

BIOVIA Materials Studio Forcite Plus is a set of tools for performing classical simulations using either molecular mechanics or molecular dynamics. It enables the researcher to calculate the energy, optimize the geometry, or study the temporal evolution of a structure containing thousands of atoms. Analysis tools and tasks enable the prediction of time-dependent properties such as diffusion, calculate mechanical properties such as Young's Modulus, predict cohesive energy density and solubility parameters, and probe structural information.
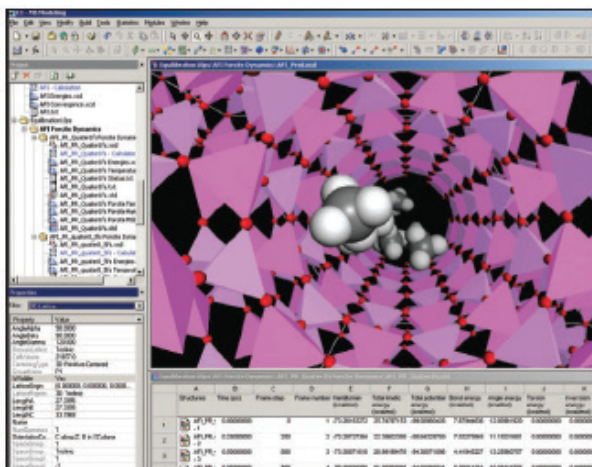

Figure 1: BIOVIA Materials Studio Forcite Plus allows you to run molecular dynamics on a wide range of systems. Here, methane is seen diffusing through a zeolite pore, typical of the organic-inorganic structures that can be studied. The trajectory document can be animated to visualize the path of diffusion and the trajectory data, such as energies and cell parameters, can be viewed in a study table.

KEY USES OF BIOVIA MATERIALS STUDIO FORCITE PLUS

Classical simulations techniques are widely used for property prediction and structure elucidation for many different types of materials.

Polymers

Using BIOVIA Materials Studio Forcite Plus with the BIOVIA BIOVIA Materials Studio Compass forcefield enables the prediction of properties such as density, diffusion, mechanical properties and solubility parameters. These enable the researcher to study problems such as molecular compatibility between polymers and small molecules, other polymers, and surfaces. Other properties such as diffusivity of small molecules in polymer matrices and glass transition temperatures can be studied.

Catalysis

Tasks in BIOVIA Materials Studio Forcite Plus such as simulated annealing enable the search for low energy sites and preoptimization of a structure prior to more accurate quantum mechanics calculations.

Zeolites

Difussion of gas molecules in zeolite frameworks can be estimated using classical simulation techniques.

Molecular Crystals

Structure optimization using high-quality forcefields such as BIOVIA Materials Studio Compass, enable the understanding of simple and complex crystalstructures

THE BIOVIA MATERIALS STUDIO ADVANTAGE

BIOVIA Materials Studio Forcite Plus is operated from within the BIOVIA Materials Studio software environment. BIOVIA Materials Studio Visualizer, the core BIOVIA Materials Studio product, offers a wide range of model building and visualization tools. You can rapidly construct models of the systems that interest you, select and run BIOVIA Materials Studio Forcite Plus—all with a few mouse clicks

To use BIOVIA Materials Studio Forcite Plus, you begin with a molecular, 2D, or 3D periodic structure of the system you want to study. All these material types can be constructed using the advanced building tools within

BIOVIA Materials Studio Visualizer.

You then choose a calculation task (such as Energy, Geometry Optimization, or Molecular Dynamics), the desired quality level for the task, and a forcefield. Clicking on Run will start an interactive calculation using the clientserver architecture.

BIOVIA Materials Studio Forcite Plus updates the active structure document and reports the results in text and chart documents. All BIOVIA Materials Studio Forcite Plus tasks can be executed in parallel using MPI to decrease your time to solution.

When the calculation is complete, all files are automatically returned to your BIOVIA Materials Studio project for analysis. The tools range from simple analysis of properties, such as the change in density or Hamiltonian during a molecular dynamics simulation, to more complex structural properties like the mean squared displacement. All of the analysis tools are available from a simple interface and the study table can be used to visualize and plot properties from a trajectory file.

You can also write scripts to control BIOVIA Materials Studio Forcite Plus, providing tight integration between BIOVIA Materials Studio Forcite Plus and other modules exposed through the MaterialsScript API. Scripting allows you to automate repetitive tasks and further customize the functionality in BIOVIA Materials Studio.

HOW DOES BIOVIA MATERIALS STUDIO FORCITE PLUS WORK?

BIOVIA Materials Studio Forcite Plus uses a classical mechanics model with atoms that cannot penetrate each other. The interactions between the atoms are defined by a forcefield which contains the parameters for all the different combinations of interactions. The interactions are defined by different functional forms which describe valence interactions, such as bond stretches and angle terms, and nonbonded interactions such as van der Waals and electrostatic interactions. The forcefield can contain as many, or few, of the different functional forms as is required to accurately describe the system of interest. As the complexity of the forcefield increases, the number of parameters required also increases. Generating good forcefield parameters is key in getting accurate results from BIOVIA Materials Studio Forcite Plus.
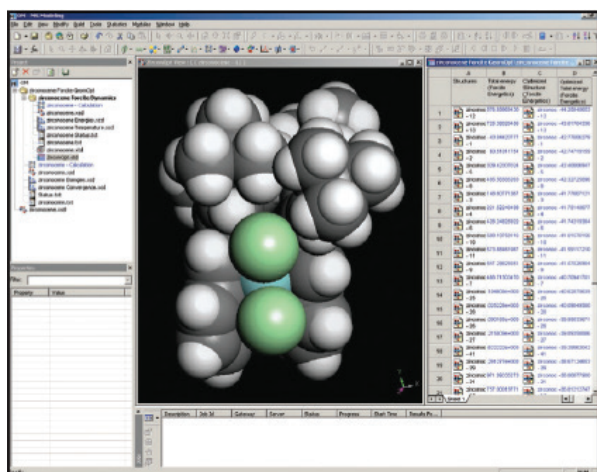

Figure 2: This zirconocene structure, an organometallic complex, has a complex energy profile. BIOVIA Materials Studio Forcite Plus, in conjuction with the study table, is used to obtain the lowest energy conformation for this structure.

A range of forcefields are supplied with BIOVIA Materials Studio Forcite Plus, including BIOVIA Materials Studio Compass for simulating condensed phase systems, and Universal for general calculations.

FEATURES AND CAPABILITIES

Energy calculations
- Calculate energy for a structure
- Support for BIOVIA Materials Studio Compass, cvff, pcff, Dreiding, Universal, and customized forcefields.
- Define charges by forcefield, using Charge Equilibration, or Gasteiger methods
- Set quality level to balance speed and accuracy
- Define non-bond interaction calculations using atom based, group based, or Ewald summation methods
- Add an electric field across a cell
- Add restraint energies to distances, angles or torsions
- Support for molecules, surfaces, and crystals

Geometry optimization
- Optimize the geometry of a structure to a low energy minima
- 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
- Cartesian atom positions may be constrained
- Define rigid bodies to limit degrees of freedom
- Optimizes all structures if a trajectory is provided

Dynamics
- Study temporal evolution of a structure
- Range of dynamics ensembles (NVE, NVT, NPT, NPH)
- Nose, Velocity Scale, Andersen, and Berendsen thermostats
- Andersen and Berendsen barostats
- Random or user specified initial velocities
- Cartesian atom positions may be constrained
- Results saved to trajectory, optionally includes forces and velocities
- Restart of dynamics with option to append to current trajectory

Quench Dynamics
- Combine geometry optimization and dynamics to sample low energy conformations

Simulated Annealing
- Perform dynamics calculations at range of different temperatures
- Control temperature ranges and number of cycles
- Optionally quench after each cycle

Confined Shar
- Shear a fluid between two surfaces
- Specify shear rate
- Requires a 3D periodic cell as input Cohesive Energy Density Calculates cohesive energy density and solubility parameter
- Calculate intramolecular energies
- Include structures in study table

Mechanical Properties

- Apply strain and calculate mechanical properties using static approach
- Calculate elastic stiffness and compliance constants
- Bulk, shear modulus, Young's modulus
- Compressibility, velocities of sound, Lame constants

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 concentration, temperature, and velocity profiles in any direction, average over frames
- Plot and analyze distances, angles and torsions
- 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
- Generate density fields for trajectories
- 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

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

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