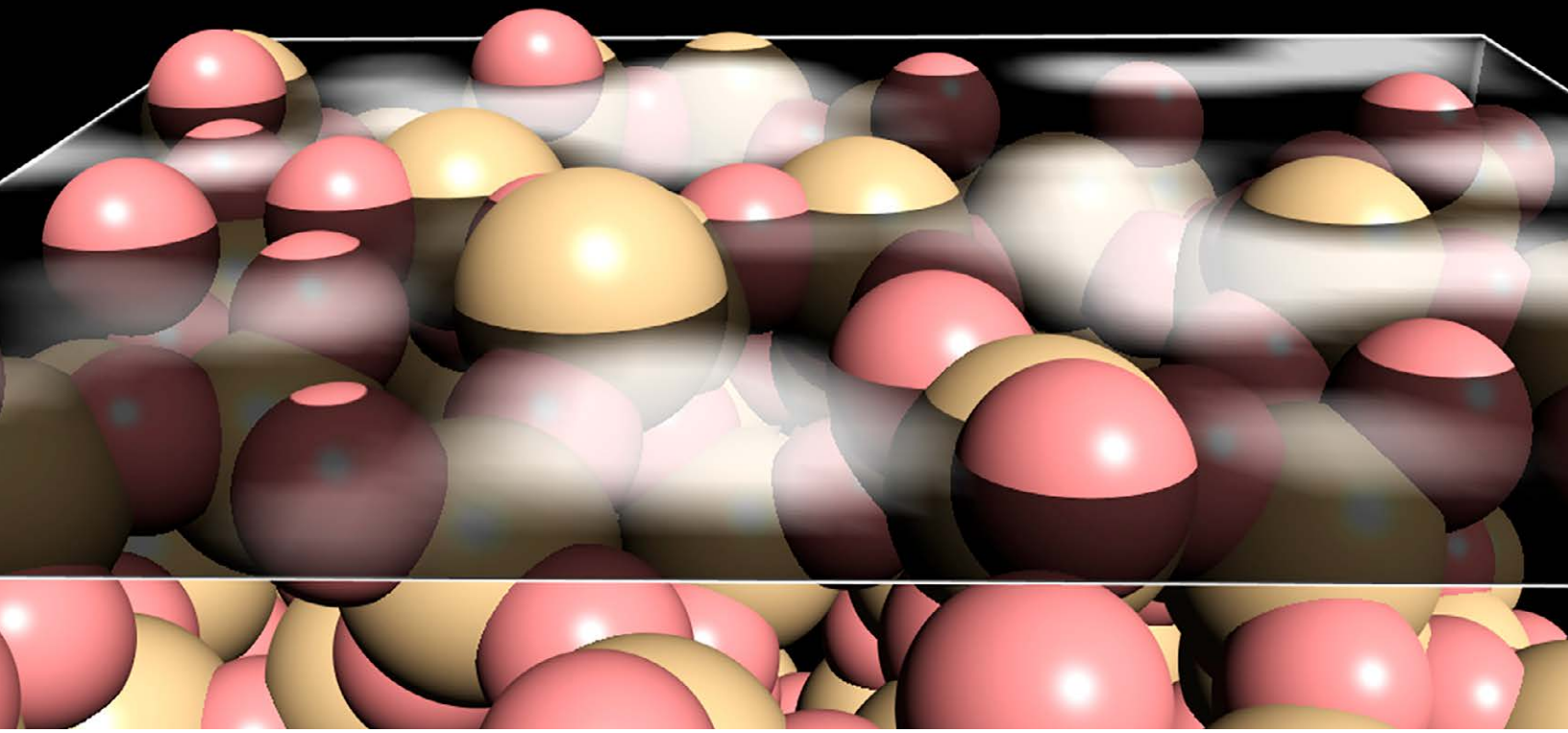
BIOVIA MATERIALS STUDIO
FORCITE PLUS

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?

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, and 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.

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 Materials Studio Forcite Plus with the 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.

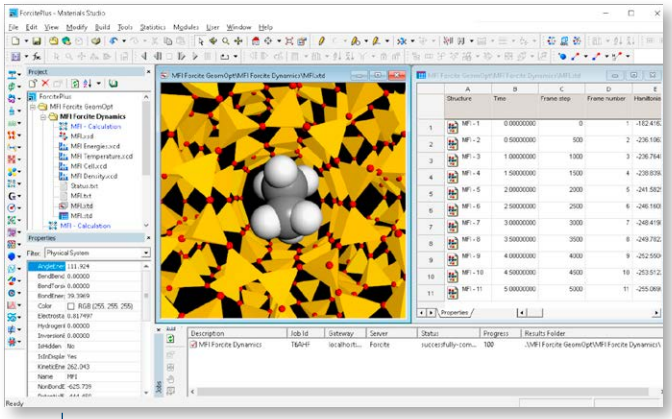


Figure 1: Materials Studio Forcite Plus allows you to run molecular dynamics on a wide range of systems. Here, ethane is seen diffusing through a zeolite pore, typical organic-inorganic structures that can be studied. The trajectory document can be animated to visualize the path of diffusion and the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

Catalysis

Tasks in 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 Materials Studio Compass, enables the understanding of simple and complex crystal structures.

THE MATERIALS STUDIO ADVANTAGE

Materials Studio Forcite Plus is operated from within the Materials Studio software environment. Materials Studio Visualizer, the core 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 Materials Studio Forcite Plus—all with a few mouse clicks

To use Materials Studio Forcite Plus, you simply 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 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.

Materials Studio Forcite Plus updates the active structure document and reports the results in both text and chart documents. All 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 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 Materials Studio Forcite Plus, providing tight integration between 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 Materials Studio.

HOW DOES BIOVIA MATERIALS STUDIO FORCITE PLUS WORK?

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 Materials Studio Forcite Plus.

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

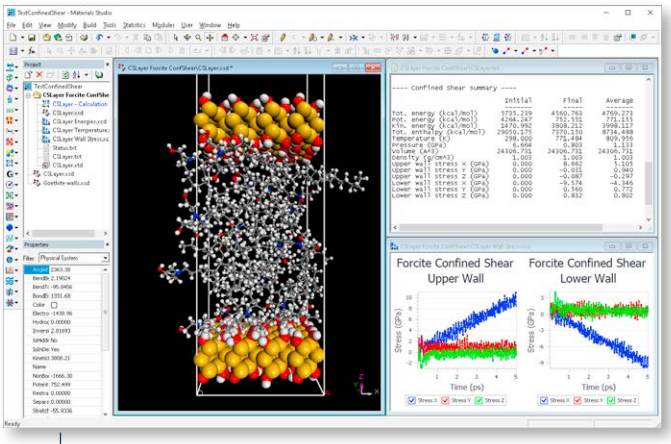


Figure 2: This model shows the input and output for a confined shear simulation using walls constructed from goethite. Confined shear is a dedicated task available in Forcite Plus.

FEATURES AND CAPABILITIES

Energy calculations

- Calculate energy for a structure
- Support for 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 nonbonded 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
- Optimize 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 Shear

- 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

Graphics Processing Unit (GPU) Support

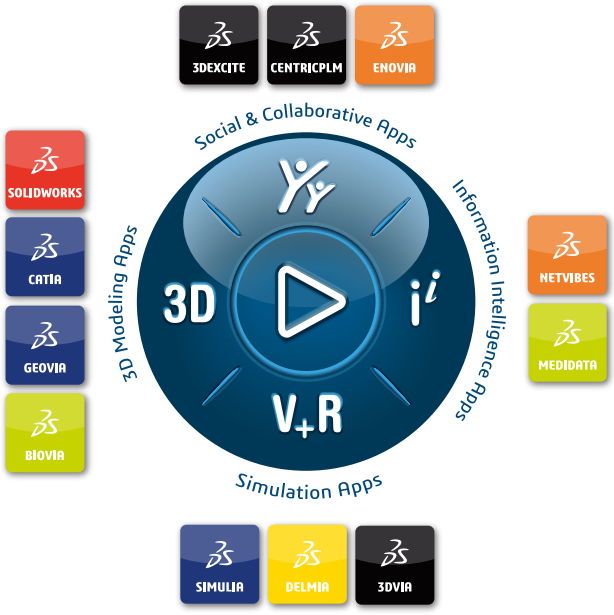
Forcite Plus can make use of NVIDIA GPUs to provide hugely accelerated molecular dynamics calculations. Please refer to the latest system requirements document for supported categories of GPUs.

LEARN MORE

Our **3D**EXPERIENCE® Platform powers our brand applications, serving 11 industries, and provides a rich portfolio of industry solution experiences.

Dassault Systèmes, the **3D**EXPERIENCE Company, is a catalyst for human progress. We provide business and people with collaborative virtual environments to imagine sustainable innovations. By creating 'virtual experience twins' of the real world with our **3D**EXPERIENCE platform and applications, our customers push the boundaries of innovation, learning and production.

Dassault Systèmes' 20,000 employees are bringing value to more than 270,000 customers of all sizes, in all industries, in more than 140 countries. For more information, visit **www.3ds.com**.



DASSAULT SYSTEMES | The **3D**EXPERIENCE® Company

Europe/Middle East/Africa
Dassault Systèmes
10, rue Marcel Dassault
CS 40501
78946 Vélizy-Villacoublay Cedex
France

Asia-Pacific
Dassault Systèmes K.K.
ThinkPark Tower
2-1-1 Osaki, Shinagawa-ku,
Tokyo 141-6020
Japan

Americas
Dassault Systèmes
175 Wyman Street
Waltham, Massachusetts
02451-1223
USA