

Molecular mechanics and dynamics simulation for structure and property prediction

Supports use of the powerful COMPASS forcefield for condensed phase simulation

Wide range of analysis tools for property prediction

Discover

Discover[®] offers powerful atomistic simulation methods that can be applied to a wide range of molecules and materials. Such simulation assists research in areas including catalysis, separations, crystallization, and polymer sciences. It explains relationships between structure and molecular behavior, provides insight into key molecular interactions, and predicts critical properties of solids, liquids, and gases.

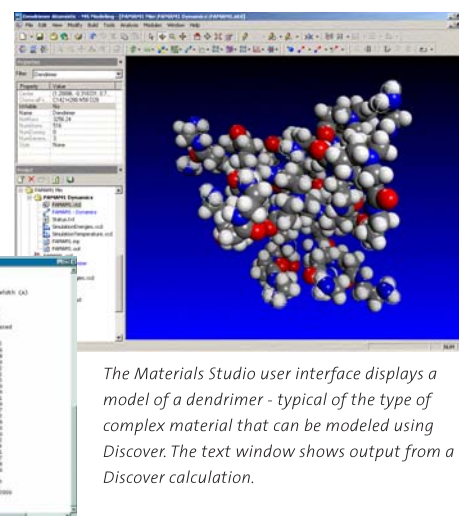
What Does Discover Do?

Discover is Materials Studio's simulation engine. It incorporates a broad spectrum of molecular mechanics and dynamics methodologies that have demonstrated applicability to molecular design. Using a carefully-derived forcefield as the foundation, minimum energy conformations, as well as families of structures and dynamics trajectories of molecular systems, can be computed with confidence.

Discover provides underlying calculations for products such as Amorphous Cell. It also supports varied simulation strategies. Periodic boundary conditions allow the simulation of solid-state systems, whether crystalline or amorphous, and of solvated systems. Comprehensive analysis features enable the extraction of pertinent results from the simulation. Features are listed overleaf. These capabilities allow you to address serious projects in computer aided molecular design.

The Materials Studio Advantage

Discover is operated from within the Materials Studio[®] software environment, that provides a user interface that is easy-to-use and quick to learn, complying with Windows[®] standards. It offers a wide range of model building and visualization tools. You can rapidly construct models of the systems that interest you, select Discover with a double mouse click, and then run an advanced simulation. A flexible client-server



The Materials Studio user interface displays a model of a dendrimer - typical of the type of complex material that can be modeled using Discover. The text window shows output from a Discover calculation.

architecture means that calculations can be run on servers located elsewhere on your network.

Results are then returned to your PC, where they may be displayed and analyzed. You can easily produce high quality graphics of molecular and materials structures. 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.

Discover, running within Materials Studio, brings some of today's most widely-used and well validated atomistic simulation technology to your desktop.

Features

User Interface and Systems

- Operated from a PC running Windows — Materials Visualizer must be installed
- Calculations can be performed on remote servers
- Standard Windows user-interface, enabling seamless data transfer to and from other PC applications.

Forcefields

- Includes validated parameterizations, such as PCFF and CVFF
- Supports plug-in of the COMPASS force field for condensed phase property prediction.

Molecular Mechanics and Dynamics

- Energy minimization of flexible geometries with a choice of optimizers, including steepest descents, conjugate gradients, quasi-Newton, Newton, and truncated-Newton methods
- Microcanonical (NVE), canonical (NVT), constant pressure (NPT), and constant enthalpy (NPH) molecular dynamics simulations
- Simulations using periodic boundary conditions supporting bonds across boundaries and full symmetry in the case of energy minimization
- Constraining selected atoms during a simulation.

Analysis

Structural

- Conformational analysis for polymers and peptides during molecular dynamics
- Calculation of the radial distribution function, orientational correlation functions and scattering curves
- Measurement of distributions of distances, angles and radii of gyration
- Concentration profiles for any desired component
- Hydrogen bonds.

Energetics

- Cohesive energy density and solubility parameter of bulk molecular systems
- Decomposition of internal (valence) energies
- Temperature profiles in non-equilibrium systems.

Mechanical

- Material elastic constants using various methods.

Dynamical Quantities

- Mean square displacements and velocity correlation functions for estimating self-diffusion coefficients
- Rotational time correlation functions
- Dipole moment correlation functions
- Space-time correlations.

Vibrational

- Calculation of vibrational intensities, as well as normal mode analysis.

Other

- Fluctuation-formula-based properties, such as thermal expansion coefficients, depending on the ensemble simulated.

Note: Additional features are available through the command-line interface to Discover. Examples include commands for direct access to most of Discover's internal data, powerful vector and geometry functions for customizing simulations, and specialized tools for manipulating dynamical pseudo atoms, tethers and restraints.

System Requirements:

For Materials Studio system requirements see www.accelrys.com/products/mstudio/sysreqs.html