DATASHEET

accelrys®

MATERIALS STUDIO OVERVIEW

Modeling and Simulation for Next Generation Materials. Materials Studio® is a complete modeling and simulation environment that enables researchers in materials science and chemistry to develop new materials by predicting the relationships of a material's atomic and molecular structure with its properties and behavior. Using Materials Studio, researchers in many industries can engineer better performing materials of all types, including pharmaceuticals, catalysts, polymers and composites, metals and alloys, batteries and fuel cells, nanomaterials, and more.

Materials Studio is the world's most advanced, yet easy to use environment for modeling and evaluating materials performance and behavior. Using Materials Studio, materials scientists experience the following benefits:

- Reduction in cost and time associated with physical testing and experimentation through "Virtual Screening" of candidate material variations.
- Acceleration of the innovation process - developing new, better performing, more sustainable, and cost effective materials faster than can be done with physical testing and experimentation.
- Improved fundamental understanding of the relationship between atomic and molecular structure with material properties and behavior.
- Powerful materials informatics capabilities through adoption of computational materials science as a complement to laboratory experimentation.
- Automation & best-practice sharing with the Materials Studio Collection for Pipeline Pilot, as well as the MaterialsScript API.

VISUALIZATION

Chemists, polymer scientists, and other materials scientists become productive faster and with less effort using Materials Studio Visualizer, the easiest to use and most complete graphical user environment for materials modeling and simulation. Materials Studio Visualizer provides capability to construct, manipulate and view models of molecules, crystalline materials, surfaces, polymers, and mesoscale structures. It also supports the full range of Materials Studio simulations with capabilities to visualize results through images, animations, graphs, charts, tables, and textual data. Most tools in the Materials Visualizer can also be accessed through the MaterialsScript API, allowing expert users to create custom capabilities and automate repetitive tasks. Materials Studio Visualizer's Microsoft Windows client operates with a range of Windows and Linux server architectures to provide a highly responsive user experience.

SOLUTION TECHNOLOGIES

Materials Studio provides a complete range of simulation capabilities from quantum, atomistic, mesoscale, statistical, analytical and crystallization tools. Its' broad range of solutions enable researchers to evaluate materials at various particle sizes and time scales in order to predict properties more accurately and evaluate performance in the shortest time possible.

QUANTUM TOOLS

Materials Studio provides a range of quantum mechanics-based tools for molecules and periodic structures, including density functional methods, linear scaling DFT, QM/MM and semi-empirical tools. These tools provide accurate results for the structural, thermophysical, electronic, and optical properties of materials.

Product	Description
CASTEP	CASTEP simulates the properties of solids, interfaces, and surfaces for a wide range of materials including ceramics, semiconductors, and metals using a plane-wave density functional method.
DMol^3	DMol^3 is used to model the electronic structure and properties of organic and inorganic molecules, molecular crystals, covalent solids, metallic solids, and infinite surfaces using DFT.
DFTB$^+$	DFTB$^+$ is a semi-empirical module for simulating electronic properties of materials. It uses a tight-binding approach based on density functional theory to enable quantum mechanical accuracy on larger system sizes.
NMR CASTEP	NMR CASTEP predicts NMR chemical shifts and electric field gradient tensors from first principles. The method can be applied to compute the NMR shifts of both molecules and solids for a wide range of materials including ceramics and semiconductors.
ONETEP	ONETEP is a linear scaling DFT code, enabling accurate, first principles calculations on systems of up to thousands of atoms.
QMERA	QMERA employs QM/MM method combining the accuracy of a quantum with the speed of a forcefield calculation. This approach makes it possible to perform accurate calculations on very large systems for substantially less effort.
VAMP	VAMP is capable of rapidly predicting many physical and chemical properties for molecular organic and inorganic systems using a semi-empirical molecular orbital method. VAMP is an ideal intermediate approach between forcefield and first principles methods.

CLASSICAL SIMULATION TOOLS

Materials Studio offers a very wide range of methods based on classical interactions between atoms and molecules. These include Molecular Dynamics, Lattice Dynamics and various Monte Carlo based methods as well as the provision of forcefields.

Product	Description
Adsorption Locator	Adsorption Locator finds low-energy adsorption sites for molecules on both periodic and non-periodic substrates.
Amorphous Cell	Amorphous Cell is a suite of computational tools that allow you to construct representative models of complex amorphous systems and to predict key properties.
Blends	Blends predicts phase diagrams and interaction parameters for liquid-liquid, polymer-polymer, and polymer-additive mixtures, phase equilibria, and separations technology.

CLASSICAL SIMULATION TOOLS (continued)

Product	Description
Conformers	Conformers provides conformational search algorithms and analysis tools to characterize molecular conformation and flexibility.
COMPASS	COMPASS is a forcefield which enables accurate prediction of structural, conformational, vibrational, and thermophysical properties for a broad range of molecules in isolation and in condensed phases, and under a wide range of conditions of temperature and pressure.
Forcite Plus	Forcite Plus offers molecular mechanics and dynamics methods for molecules and periodic systems. The tool includes a wide range of analysis features to predict mechanical properties, diffusivity, local structure, density variations, cohesive energy density, dipole autocorrelation functional and more. Supported forcefields are COMPASS, CVFF, PCFF, Dreiding, and Universal.
GULP	GULP is a method for optimization, property calculation and dynamics of materials. It includes a wide range of forcefields for metals, oxides, minerals semiconductors, as well as molecular mechanics forcefields for covalent systems. Forcefield fitting tools are also provided to develop parameters for custom materials.
Sorption	Sorption provides a means of predicting fundamental properties needed for investigating adsorption and separations phenomena, such as sorption isotherms and Henry's constants.

MESOSCALE SIMULATION TOOLS

Mesoscale methods in Materials Studio are based on a coarse-graining approach, whereby groups of atoms are replaced by beads. These methods enable the modeling of behavior at length and time scales which are beyond the range of classical tools.

Product	Description
MesoDyn	MesoDyn is a classical density functional method for studying the long length- and time-scale behavior of complex fluid systems, in particular the phase separation and structure of complex polymer systems.
Mesocite	Mesocite is a coarse-grained simulation module for the study of materials at length scales ranging from nanometers to micrometers and time scales from nanoseconds to microseconds. Mesocite can provide structural and dynamic properties of fluids in equilibrium, under shear or in confined geometries.

STATISTICAL TOOLS

Statistical tools are ideal to screen compounds quickly by relating molecular traits directly to experimentally observed quantities.

Product	Description
QSAR	QSAR's (Quantitative Structure-Activity Relationships) integration in Materials Studio provides access to a wide range of descriptors and advanced analysis capabilities to help generate high quality structure activity relationships. QSAR includes a wide range of descriptors including topological and electro-topological descriptors. Also, Jurs descriptors enable charge distribution on solvent surfaces to be examined; VAMP Descriptors further extend the range of 3D descriptors into those including electronic interactions; and GFA applies a sophisticated genetic algorithm method to calculate quantitative structure-activity relationships.
QSAR Plus	QSAR Plus adds the power of the DMol3 Descriptors for calculating reactivity indices and accurate energies to QSAR. Also included are Neural Networks to build non-linear models and models that are more resistant to noisy datasets than other model building methods. It can also be used with datasets that have some missing values, and can be used to build weighted models to predict multiple physical properties.
Synthia	Synthia calculates properties of homo- and copoplymers using advanced Quantitative Structure-Property Relationships (QSPRs). It allows researchers to rapidly screen candidate polymers for a wide range of properties.

ANALYTICAL & CRYSTALLIZATION TOOLS

Analytical and crystallization tools are employed to investigate, predict, and modify crystal structure and crystal growth.

Product	Description
Morphology	Morphology allows you to predict crystal morphology from the atomic structure of a crystal. Morphology allows for the prediction of crystal shape, the analysis of crystal surface stability, the development of tailor-made additives, and the control of solvent and impurity effects.
Polymorph Predictor	Polymorph Predictor allows you to predict potential polymorphs of a given compound directly from the molecular structure.
Polymorph	Predictor has been developed for use with fairly rigid, non-ionic or ionic molecules composed primarily of carbon, nitrogen, oxygen, and hydrogen. The approach is based on the generation of possible packing arrangements in all reasonable space groups to search for the low-lying minima in lattice energy.
Motif	Motif analyzes connectivity information in molecular crystals, providing a qualitative and quantitative analysis method of hydrogen bond topologies. Combined with the predictive capabilities of Materials Studio Polymorph, Motif allows for categorization and statistical scoring of proposed structures. It interfaces with the Cambridge Structural Database exploiting Cambridge Crystallographic Data Centre's Mercury functionality.
Reflex	Reflex simulates X-ray, neutron, and electron powder diffraction patterns based on models of crystalline materials. Reflex Plus offers a complete package for the determination of crystal structures from medium- to high-quality powder diffraction data.
Reflex QPA	Reflex QPA extends the Reflex functionality for quantitative phase analysis, allowing for the determination of the relative proportion of different phases, including both inorganic as well as organic systems, in a mixture based on powder diffraction data.
X-Cell	X-Cell is an efficient, indexing algorithm for medium- to high-quality powder diffraction data. X-Cell uses an extinction-specific dichotomy procedure to perform an exhaustive search of parameter space to establish a complete list of all possible unit cell solutions.

To learn more about Materials Studio, go to

accelrys.com/materials-studio