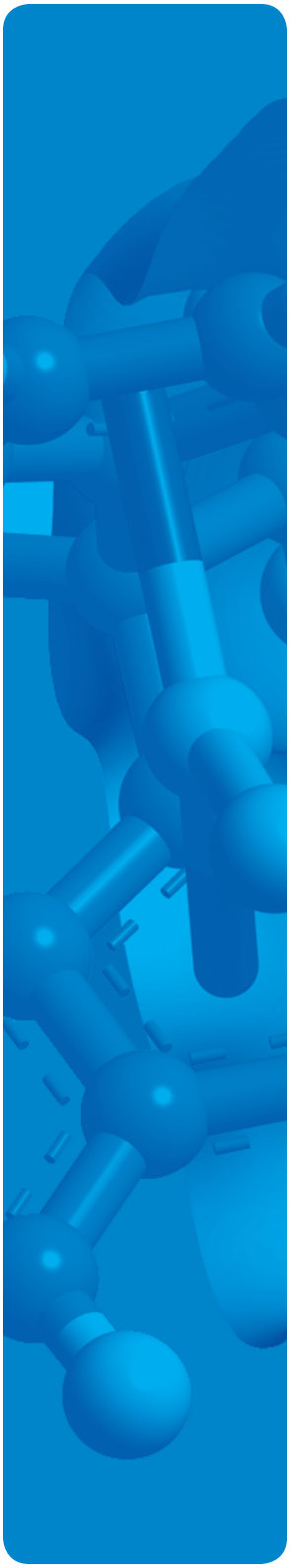
MATERIALS STUDIO

Materials Science Modeling & Simulation

Materials Studio Product Descriptions



Materials Studio® is a software environment that brings the world's most advanced and validated materials simulation technology to desktop computing, solving key problems throughout the R&D process.

Materials Studio offers access to the complete range of computational materials science methods via desktop computing. It is designed for structural and computational researchers in chemicals and materials R&D who need to perform expert-level modeling and simulations tasks in an easy-to-learn yet powerful environment. It provides tools for modeling crystal structure and crystallization processes, for the study of polymer properties, catalysis, and the study of structure-activity relationships.

Analytical & Crystallization

Product	Description
Conformers	Conformers provides conformational search algorithms and associated analysis tools, allowing you to characterize molecular conformation and flexibility, and gain insight into geometric and energetic properties.
GULP	GULP is a forcefield method with a wide range of materials forcefields, from shell model for ionic systems, embedded atom for metals, bond order potentials for semiconductors and nanotubes, to molecular mechanics forcefield support for covalent systems. Apart from optimization and dynamics, GULP is able to calculate a wide range of properties, including mechanical, electric, lattice, and thermodynamic quantities. GULP can be used for a range of system types such as molecules and cluster, surfaces, and bulk systems.
Materials Visualizer	Materials Visualizer provides all of the tools that you require to construct graphical models of molecules, crystalline materials, and polymers. You can manipulate, view, and analyze these models. Materials Visualizer also handles graph, tabular, and textual data and provides the software infrastructure and analysis tools to support the full range of Materials Studio's products.
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 via inter-molecular interactions within a bulk crystal, the development of tailor-made additives, and the control of solvent and impurity effects. Morphology's application areas include pharmaceuticals, agrochemicals, food sciences, petrochemicals, cements, and commodity and specialty chemicals.
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 polymorph prediction of fairly rigid, non-ionic or ionic molecules composed mostly 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.
Reflex	Reflex simulates X-ray, neutron, and electron powder diffraction patterns based on models of crystalline materials. Reflex aids the determination of crystal structure, assists the interpretation of diffraction data, and is applied to validate the results of experiment and computation.
Reflex Plus	Reflex Plus is an advanced version of Reflex, adding the extensively validated Powder Solve technology to the standard Reflex functionality. Reflex Plus offers a complete package for the determination of crystal structures from medium- to high-quality powder diffraction data.

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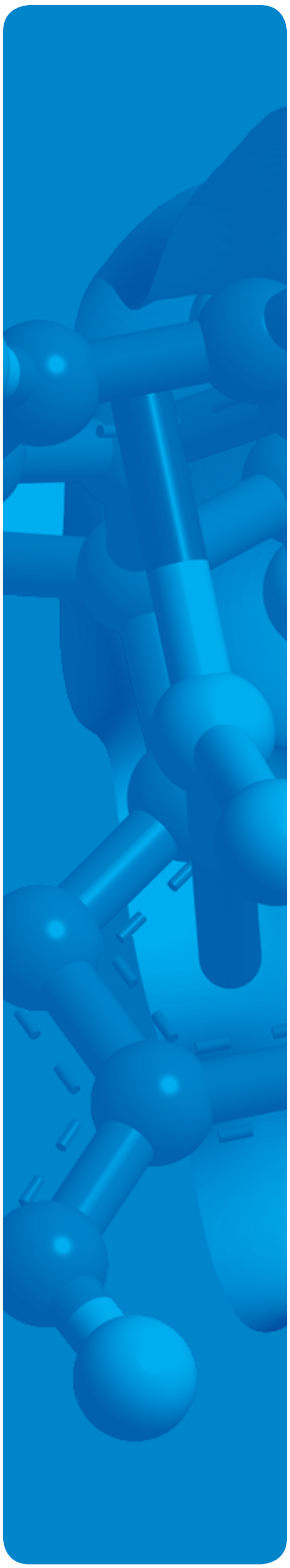


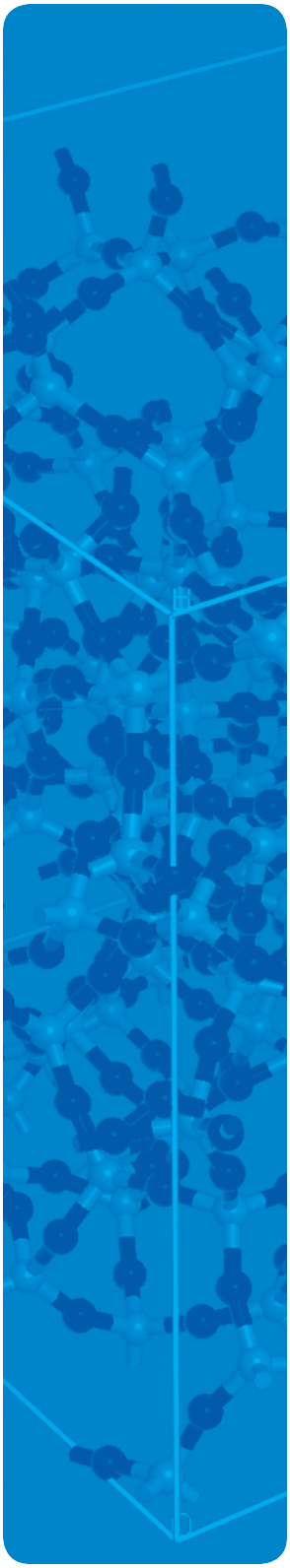
Analytical & Crystallization

Product	Description
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. It is a widely used analytical method for phase characterization in various industries.
X-Cell	X-Cell is a novel, robust, efficient, integrated, and easy-to-use indexing algorithm for medium- to high-quality powder diffraction data obtained from X-ray, neutron, and electron radiation sources. 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.

Polymers & Simulations

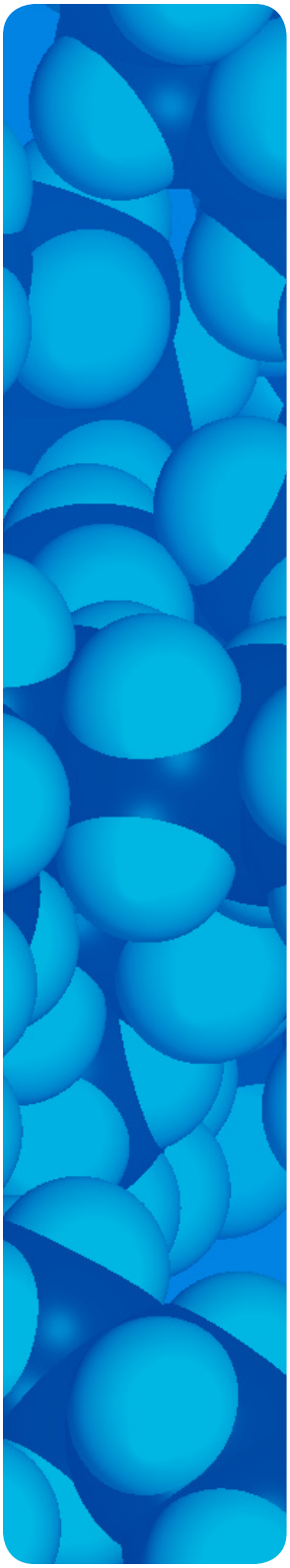
Product	Description
Amorphous Cell	Amorphous Cell is a suite of computational tools that allow you to construct representative models of complex amorphous systems and to predict key properties. By observing the relation between system structure and properties, you can obtain a more thorough understanding of the important molecular features, allowing you to better design new compounds or new formulations. Among the properties that you can predict and investigate are cohesive energy density, equation-of-state behavior, chain packing, and localized chain motions.
Blends	Blends predicts phase diagrams and interaction parameters for liquid-liquid, polymer-polymer, and polymer-additive mixtures, for studying the structural factors affecting the behavior of blends and formulations. Applications include calculating the free energy of mixing of two polymers, obtaining the binodal and spinodal curve in the mixing of two liquid crystals, determining the adhesion strength of a new epoxy on a carbon fiber, and studying delamination problems in a multilayered material as a function of temperature. Blends aids the study of the compatibility of polymer blends and additives, formulation work, solvent effects on polymers, polymer adhesion, partition coefficients, liquid-liquid phase equilibria, and separations technology.
Conformers	Conformers provides conformational search algorithms and associated analysis tools, allowing you to characterize molecular conformation and flexibility, and gain insight into geometric and energetic properties.
COMPASS	COMPASS stands for Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies. It is the first ab initio forcefield that has been parameterized and validated using condensed-phase properties in addition to various ab initio and empirical data for molecules in isolation. Consequently, this force field enables accurate and simultaneous 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.

Polymers & Simulations



Product	Description
Discover	Discover offers powerful atomistic simulation methods that can be applied to a wide range of molecules and materials. Atomistic 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 important properties of solids, liquids, and gases.
DPD	DPD (Dissipative Particle Dynamics) is a state-of-the-art mesoscale simulation method for the study of complex fluids. Such fluids pervade industrial research from paints to pharmaceuticals and from cosmetics to the controlled release of drugs. DPD can provide structural and dynamic properties of fluids in equilibrium, under shear or confined to narrow cavities, at length and time-scales beyond the scope of traditional atomistic molecular dynamics simulation methods.
Equilibria	A Monte Carlo Gibbs Ensemble-based program for the determination of phase diagrams of single molecules, binary, and ternary systems. It includes the NERD force field with Coulombic interaction terms and parameters for a range of organic groups.
Forcite	A molecular mechanics product for energy calculation and geometry optimization of molecules and periodic systems. Forcite calculations strictly honor any crystal symmetry. Supported force fields are COMPASS, CVFF, PCFF, Dreiding, and Universal.
Forcite Plus	Forcite Plus extends the classical simulations tools of Forcite to include molecular dynamics and analysis tools. It allows the prediction of diffusivity, local structure, density variations, and dipole autocorrelation functionals.
Materials Visualizer	Materials Visualizer provides all of the tools that you require to construct graphical models of molecules, crystalline materials, and polymers. You can manipulate, view, and analyze these models. Materials Visualizer also handles graph, tabular, and textual data and provides the software infrastructure and analysis tools to support the full range of Materials Studio's products.
MesoDyn	MesoDyn is a dynamic simulation method for studying the long length and time behavior of complex fluid systems, including polymer melts and blends. It has gained wide respect in literature and commercial circles with scientifically astute algorithms aimed at elucidating industrially important mesoscale structure and kinetics. Such structures are found to critically affect the bulk properties of a material and are often frozen-in by processing where timescales may be of the same order as relaxations.
Synthia	Synthia calculates polymer properties using advanced Quantitative Structure-Property Relationships (QSPRs). It allows researchers to rapidly screen candidate polymers for a wide range of properties, and allows the property prediction of copolymer blends.

Quantum & Catalysis



Product	Description
CASTEP	CASTEP is an ab initio quantum mechanical program employing density functional theory (DFT) to simulate the properties of solids, interfaces, and surfaces for a wide range of materials including ceramics, semiconductors, and metals. First principle calculations allow researchers to investigate the nature and origin of the electronic, optical, and structural properties of a system without the need for any experimental input other than the atomic number of mass of the constituent atoms.
Conformers	Conformers provides conformational search algorithms and associated analysis tools, allowing you to characterize molecular conformation and flexibility, and gain insight into geometric and energetic properties.
DMol^3	DMol^3 combines computational speed with the accuracy of quantum mechanical methods to predict materials properties both reliably and quickly. Extremely versatile and can be applied to research problems in chemistry, materials science, chemical engineering, and solid state physics.
GULP	GULP is a forcefield method with a wide range of materials forcefields, from shell model for ionic systems, embedded atom for metals, bond order potentials for semiconductors and nanotubes, to molecular mechanics forcefield support for covalent systems. Apart from optimization and dynamics, GULP is able to calculate a wide range of properties, including mechanical, electric, lattice, and thermodynamic quantities. GULP can be used for a range of system types such as molecules and cluster, surfaces, and bulk systems.
Materials Visualizer	Materials Visualizer provides all of the tools that you require to construct graphical models of molecules, crystalline materials, and polymers. You can manipulate, view, and analyze these models. Materials Visualizer also handles graph, tabular, and textual data and provides the software infrastructure and analysis tools to support the full range of Materials Studio's products.
NMR CASTEP	NMR CASTEP predicts key magnetic resonance properties of molecules and solid state materials from first principles. Based on density functional theory (DFT), NMR CASTEP provides a means to compute NMR chemical shifts and electric field gradient tensors with unprecedented accuracy. The method can be applied to compute the NMR shifts of molecules, solids, interfaces, and surfaces for a wide range of materials including organic molecules, ceramics, and semiconductors.
Sorption	Sorption provides a means of predicting fundamental properties needed for investigating adsorption and separations phenomena, such as sorption isotherms (or loading curves) and Henry's constants.
VAMP	VAMP is a semi-empirical molecular orbital package for molecular organic and inorganic systems. VAMP is an ideal intermediate module between force-field and first principles methods and is capable of rapidly calculating many physical and chemical molecular properties. VAMP is optimized to be numerically stable and fast, enabling most calculations to be run interactivewly on a PC.

Visualization & Statistics

Product	Description
QSAR	QSAR (Quantitative Structure-Activity Relationships) is a workflow solution for chemicals and materials discovery. It enables researchers to identify compounds with optimal physicochemical properties. QSAR's integration in Materials Studio provides unsurpassed access to descriptors and advanced analysis capabilities to help you to create superior materials, faster. QSAR now includes FAST Descriptors that include topological descriptors such as Chi, Kappa, and e-state keys. Also, Jurs descriptors enable charge distribution on solvent surfaces to be examined; VAMP Descriptors that further extend the range of 3D descriptors into those including electronic interactions; and GFA (Genetic Function Approximation) that apply a sophisticated genetic algorithm method to calculate quantitative structure-activity relationships (QSARs).
QSAR Plus	QSAR Plus combines the power of the DMol^3 Descriptors for calculating reactivity indices and accurate energies, with a new model building tool, Neural Networks. Neural Networks allows you 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 with some missing values, and allows you to build weighted models to predict multiple physical properties.
Materials Visualizer	Materials Visualizer provides all of the tools that you require to construct graphical models of molecules, crystalline materials, and polymers. You can manipulate, view, and analyze these models. Materials Visualizer also handles graph, tabular, and textual data and provides the software infrastructure and analysis tools to support the full range of Materials Studio's Materials Studio products.

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