MATERIALS STUDIO

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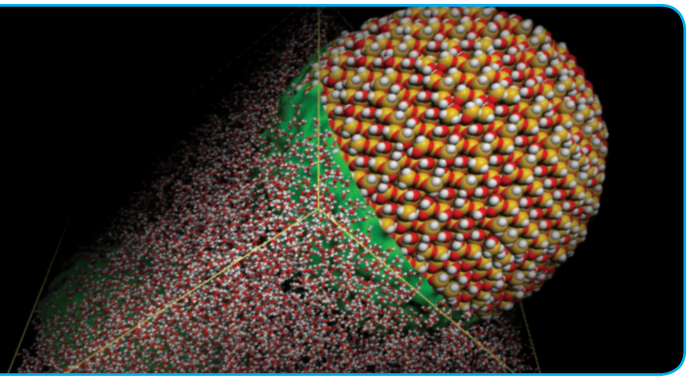
What's New in Materials Studio 5.0



Materials Studio transforms the way that researchers in chemistry, physics and materials science work to deliver breakthrough results. Materials Studio 5.0 incorporates highly efficient parallel codes and supports a wider range of polymer and instrument simulations, delivering the industry's fastest time-to-solution for sophisticated modeling tasks. With this latest release, scientists can explore a wider design space and make better informed decisions in research on catalysts, polymers, specialty chemicals and advanced materials.

Materials Studio 5.0 delivers both new and enhanced tools that enable you to get to solutions faster. Parallelization of the core classical simulations tools, Forcite Plus and Mesocite, drastically decreases calculation time. ONETEP, the linear scaling DFT module, has also seen major performance improvements. A new Amorphous Cell tool enables building of a much wider range of systems with more flexibility. With CASTEP you can now determine Raman Spectra. Developments in the Nanotechnology Consortium have focused on extending the ability to model longer length and time scales with methods such as DFTB and Kinetic Monte-Carlo.

New functionality is exposed through MaterialsScript, enabling automation of tasks and minimizing the time needed to set up calculations.

Transforming Materials Modeling.

- Efficiently Parallelized Forcite and Mesocite Modules
- Automated Polymer Workflows with MaterialsScript
- Dramatically improved ONETEP performance

Quantum Mechanics and Catalysis

CASTEP Enhancements

Raman spectroscopy

Predict Raman frequencies and intensities for solid-state materials and molecules. Characterize materials *in silico* and compare with *in situ* spectra to identify materials present.

Integration with MaterialsScript

Use MaterialsScript to automate CASTEP calculations or integrate with other Materials Studio modules. Perform complex workflows to optimize materials for catalytic, electronic, or optical applications.

VAMP Enhancement

Extended AM1* parameters

The applicability domain has been extended with a larger coverage of elements in the AM1* Hamiltonian including V, Cr, Mn, Fe, Co, Au, Br, and I.

QMERA Enhancements

Support for periodic systems using the QMPot approach enables the simulation of heterogeneous catalysis systems such as zeolites with periodic boundary conditions. QMERA now also includes vibrational frequency calculations.

DMol^3 Enhancement

Parallel performance

Improved parallel performance for vibrational frequencies using a coarse-grained parallel approach.

ONETEP Enhancement

Performance improvements

Benefit from much improved solution times with calculations running between 3 to 10 times faster.

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Classical Simulations

Amorphous Cell Enhancements

The new Amorphous Cell module makes the construction of complex condensed phase models straightforward and fast.

Improved forcefield support

Build amorphous cells of any material using any of the Forcite supported forcefields.

New packing task

Pack molecules into a cell of any shape, into cells already containing a structure, or into isosurfaces such as the interior of a nanotube to build complex structured systems.

Flexible torsion assignment

This features ensures that polymers are packed in a controlled and efficient way. You set the flexibility of your molecules, using backbone, all, or customized torsions for example to pack branched polymers into a cell.

Automate calculations

Use MaterialsScript to automate Amorphous Cell construction and packing tasks. You can combine this with Forcite Plus to build entire polymer workflows.

Forcite Plus and Mesocite

Parallel and 64-bit Linux support

Experience major performance enhancements from running jobs in parallel. The 64-bit Linux support gives the ability to take full advantage of high speed interconnects, further improving performance.

Run Forcite and Mesocite functionality in parallel from MaterialsScripts and drastically decrease calculation times.

Mesocite

Dissipative Particle Dynamics thermostat

With the implementation of a DPD thermostat into Mesocite, you can run DPD calculations in parallel, and use MaterialsScript to automate DPD workflows.

Set up calculations using reduced units and obtain results in physical units.

GULP

Set up and analyze Phonon Dispersion and Density of States calculations. Visualize and specify a reciprocal space path using the new Brillouin zone visualization.

Visualization

Brillouin zone visualization

Streamline your setup and analysis of solid state property calculations by displaying the Brillouin zone. Create paths in k-space to highlight high-symmetry lines and points.

MaterialsScript extensions

Create trajectories from MaterialsScript and delete and rename documents in the project.

Access new trajectory properties such as stress and use new tools to find and impose symmetry on structures.

Nanotechnology Consortium

Kinetix - New!

New kinetic Monte Carlo application

Kinetix bridges the gap from atomistic simulations to reaction engineering in the catalysis, adhesives and coatings area. The module employs kinetic Monte Carlo methods to simulate surface processes such as heterogeneous catalysis on time scales up to minutes.

QMERA Enhancements

Transition state searching

Reaction transition states in large systems such as zeolites can now be identified using a nudged elastic band technique within this QM/MM method.

Support for periodic QM regions

Interfaces and layers with laterally periodic QM and MM regions can now be modeled, allowing applications to self-assemble monolayers and sensor systems.

DFTB+ Enhancements

Band structures

Set up and analyze band structure calculations with DFTB+.

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