DATASHEET

WHAT'S NEW IN MATERIALS STUDIO 7.0

More Science. More Applications. More People.

Materials Studio 7.0 is the latest release of Accelrys' complete modeling and simulation environment for researchers in materials science and chemistry. Materials Studio empowers researchers to predict and understand the relationships of a material's atomic and molecular structure with its properties and behavior.

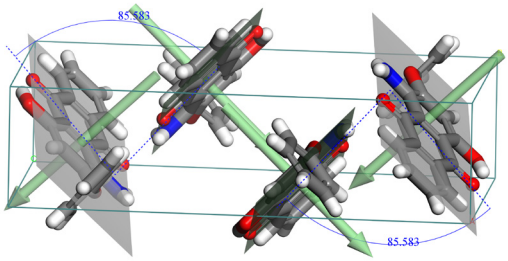
Using Materials Studio 7.0, scientists can model and evaluate materials performance and behavior as an integral part of a scientific innovation lifecycle management strategy.

MORE SCIENCE

Advancements in solubility property prediction, new forcefield types and improved electron transport lead the way in providing new science to modelers. Faster core performance enables faster, more accurate studies.

MORE APPLICATIONS

More science enables more applications for many industries. New solubility property predictions can accelerate the development of a wide range of consumer and commercial products such as specialty chemicals, coatings and consumer goods including better food and drink mixes, detergents and pills. Extended forcefields enable scientists to study a wider range of materials with greater accuracy. Understanding properties



of electronic materials such as organic light-emitting diodes enables scientists to study additional materials in areas such as electronics and fuel cell development.

MORE PEOPLE

New script functionality and continued integration with the Accelrys Enterprise Platform (AEP) and Pipeline Pilot scientific workflow authoring application enable scientists to quickly create and deploy new applications to other team members. Integration with AEP also improves collaboration in materials engineering by enabling computational experts to share best practice tools, models, methods and results with others.

* Pipeline Pilot and the Accelrys Enterprise Platform are not included for academic customers

MATERIALS STUDIO 7.0 HIGHLIGHTS

Quantum Mechanics

New functionality

- Calculate electron transport properties such as transmission and current-voltage curves using DFTB+.
- Use the TS Confirmation task in CASTEP to improve understanding of reaction pathways.
- Calculate excitation energies for molecules in a box using CASTEP and optimize the excited states.
- Study the response of a molecule or surface to an electric field using DFTB+ or CASTEP

New properties

- Calculate elastic constants and mechanical properties using DMol^3.
- Improve characterization of materials by calculating partial Density of States and vibrational modes using DFTB+

Enhanced performance

- DMol3 scaling has been dramatically improved, so that performance improves on larger numbers of cores. Wall clock times for geometry optimizations of molecular crystals have also decreased.
- Calculations using DFTB+ on small systems have been accelerated and large systems can now run in MPI parallel

Classical Simulations

New properties

- Calculate free energy of solvation using Forcite Plus.
- Estimate relative diffusion of large molecules in Forcite Plus by applying a constant force.
- Calculate thermal conductivity for amorphous materials using GULP

New functionality

- Apply an anisotropic stress using the Souza-Martins barostat or use it to calculate stress-strain curves with Forcite Plus or Mesocite.

Enhanced coverage

- A new forcefield, COMPASS II, has been added to the classical simulations tools. The coverage includes all the original COMPASS parameters but has been extended to include ionic liquids and heterocyclic molecules.

Enhanced performance

- Use the Particle-Particle-Particle Mesh Ewald method for calculating electrostatic contributions in Forcite Plus or Mesocite to give much faster calculations for large charged systems.

Visualization and Collaboration

New functionality

- Build electrodes or cleave them from existing structures. Use them to build transport devices for electron transport calculations.
- Calculate angles between planes and distances between points and planes

Enhanced usability

- Set up calculations using the module dialogs and copy the settings to a MaterialsScript. This enables fast and error-free generation of MaterialsScript and is also applicable to many of the Materials Visualizer tools. Use it to create custom components for Pipeline Pilot.
- Structures, trajectories and study tables can be exported as old formats, back to Materials Studio 5.0, for sharing and improved group collaboration.
- Text files are compressed for file transfer between client and server. Job Explorer can be refreshed.
- On-line Help is now browser-based, so multiple pages can be opened in different tabs. On-line Help can be open independent of Materials Studio.

To Learn more about Materials Studio 7.0, go to **accelrys.com/materials-studio**.