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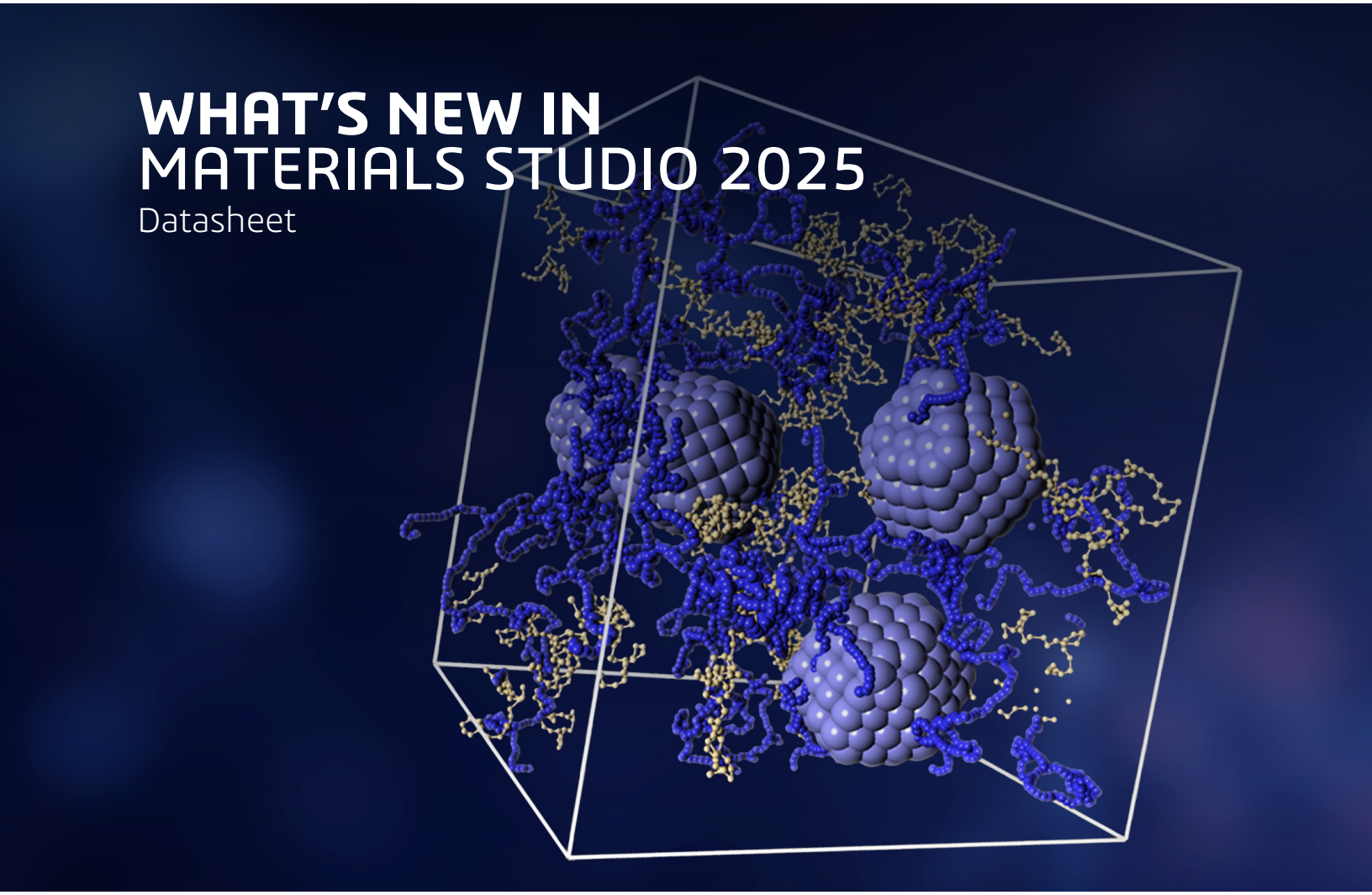
WHAT'S NEW IN MATERIALS STUDIO 2025

Datasheet



BIOVIA Materials Studio 2025 is the latest release of BIOVIA's predictive science tools for chemistry and materials science research. Materials Studio empowers researchers to understand the relationships between a material's molecular or crystal structure and its properties. Scientists using BIOVIA Materials Studio 2025 have access to an extensive suite of world-class solvers and parameter sets operating from quantum to microscales.

This release contains a range of enhancements, including new tools for building and parameterizing material models at the mesoscale, and new parameter sets for quantum and classical simulations. The introduction of MACE machine-learned forcefields to the Forcite module significantly expands the range of systems that can be studied with molecular dynamics at quantum accuracy.

With these advances, combined with enhanced performance on GPU processors, you can simulate more material properties, more accurately and more quickly than ever before.

DASSAULT SYSTEMES

BIOVIA MATERIALS STUDIO 2025 MACE LEARNED POTENTIALS

Materials Studio 2025 introduces BIOVIA Materials Studio MACE Learned Forcefields module offering a new paradigm in the choice of parameter sets for use in classical simulations. With MACE Learned potentials you can combine accuracy and performance efficiency to provide insight and property predictions for a wider range of materials.

Machine Learned Forcefields

Machine-learned forcefields are an emerging class of tools for running classical simulations that model the interactions between atoms and molecules. Traditional forcefields, such as those based on classical physics principles (e.g., Lennard-Jones potentials, Coulomb interactions), rely on predefined mathematical forms to represent the potential energy of atomic systems. These representations are simplifications that may not capture the full complexity of molecular systems, particularly for materials of unusual composition or chemistry. Additionally, the majority of generalized forcefields do not model chemical reactions between atoms at all.

Machine-learned forcefields leverage the power of machine learning algorithms to create models that predict interatomic interactions directly from data. The training data is typically quantum mechanical calculations (such as density functional theory (DFT) or coupled-cluster methods), which offer a more accurate description of electronic interactions but are computationally expensive. By using a large set of quantum data, ML algorithms can generate highly accurate forcefields that describe the potential energy surface of molecular systems, thereby improving the predictions of molecular behaviour in simulations.

MACE Learned Forcefields

Use of MACE (message passing or multi-atomic cluster expansion), as with all machine-learned approaches to atomic interaction generation, is motivated by the desire to increase computational efficiency without compromising the accuracy of the potential energy surface (PES) representing the system. MACE uses an extension of the atomic cluster expansion (ACE) approach [1] to learn the relationship between atomic configurations and the PES based on a dataset of quantum mechanical calculations. During parameterization, a neural network is trained to map atomic environments to potential energy values and forces, effectively learning how atoms interact within the system. The neural network provides a flexible representation of the PES without relying on predefined functional forms for the interactions. MACE augments traditional graph neural network features to efficiently incorporate high-body-order characteristics of the local environment around each atom, enabling predictions for systems not explicitly included in the training dataset [2][3]. MACE has emerged as a leading approach with a specific focus on improving performance and transferability.

The absence of assumptions about bonding arrangements in molecules means that chemical bonding changes in reactive systems can, in principle, be automatically included. This capability is not possible with traditional forcefields unless specifically parameterized for certain reactions. This new approach promises to significantly speed up the time to solution when investigating new materials without prior knowledge of chemical mechanisms.

FEATURES AND CAPABILITIES

Run classical molecular dynamics and evaluate configurational energy using the Forcite module with the following forcefields. Use the full range of Forcite simulation and analysis tools and Materials Studio Visualization features on the results.

MACE-OFF23

- You can use MACE-OFF23 [4] with closed-shell organic molecules. Training data used density functional theory methods for a large set of molecules containing the elements H, C, O, N, P, S, F, Cl, Br, and I.

Highlights include predictions of

- Sublimation energies comparable with use of DFT with dispersion corrections
- Robust and accurate dihedral scans
- Vibrational and thermal properties of molecular crystals
- Unit cell dimensions within 5%

MACE-MP0

- You can use versions of the foundation model MACE-MP0 [3], trained on a public database of 150k inorganic crystals - designed to give as complete as possible coverage of the periodic table. Highlights include:
- Stable molecular dynamics on wide range of molecules and materials
- Chemical reactions automatically included

Please refer to original publications for specific performance comparisons of the listed forcefields.

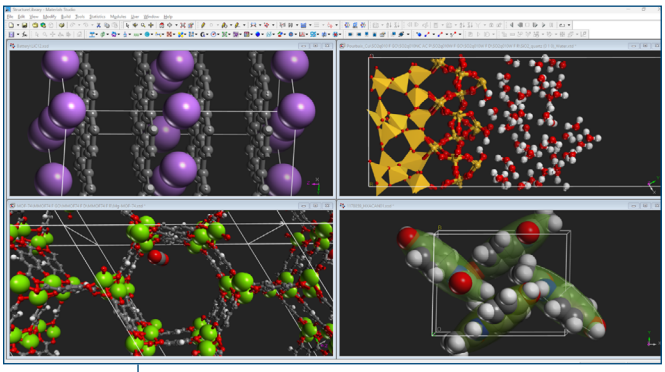


Figure 1: Materials Studio MACE Learned Forcefields can simulate a diverse range of materials models to provide insights and property predictions.

With Materials Studio 2025 you can build, simulate, analyse complex multicomponent reactive systems using machine learned forcefields.

BIOVIA MATERIALS STUDIO 2025 FOR ADVANCED MODEL BUILDING

At the start of any simulation workflow are tasks to build representative model input. Materials Studio Visualizer already provides a large array of advanced tools to construct molecules, bulk materials, interfaces and composites. Materials Studio 2025 extends these further including a new dedicated amorphous builder for mesoscale systems in the Mesocite module.

Mesocite Builder

The new Mesocite Builder helps you construct mesoscale amorphous cells using mesomolecules and Mesocite forcefields. The Mesocite Builder exploits Mesocite energy and geometry optimization calculations with forcefields based on bead-based structures. You can access the new Mesocite Builder functionality from the Materials Visualizer and MaterialsScript through new Construction, Packing, and ConfinedLayer tasks. The conformations sampled allow construction of models that start much closer to reality, reducing the time needed for equilibration.

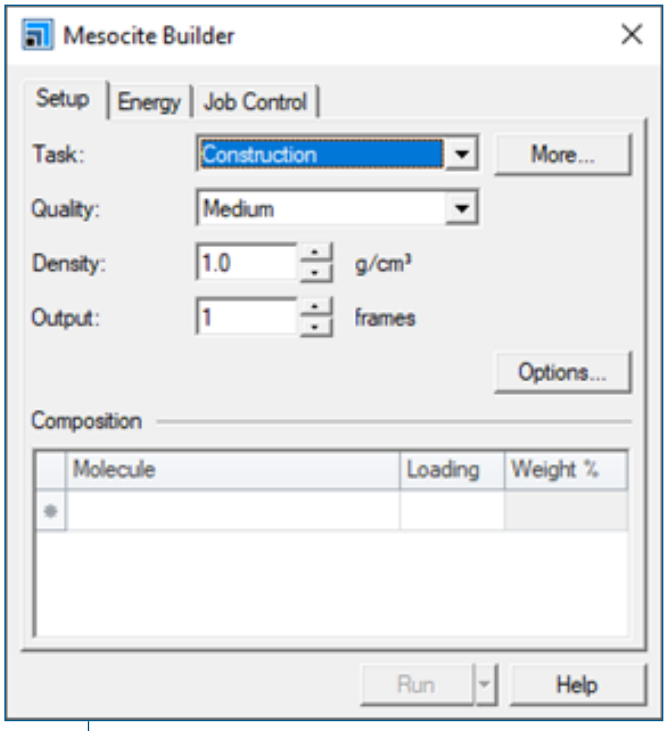


Figure 2: Materials Studio Mesocite Builder dialog showing new Construction task available.

- **New Option!** A new randomize conformation option for building mesomolecules
- **New Tutorial!** A new tutorial teaches you how to build a mesoscale amorphous cell using bead-based mesomolecules.
- **New Tasks!** New Construction, Packing, and ConfinedLayer tasks that use mesomolecules.

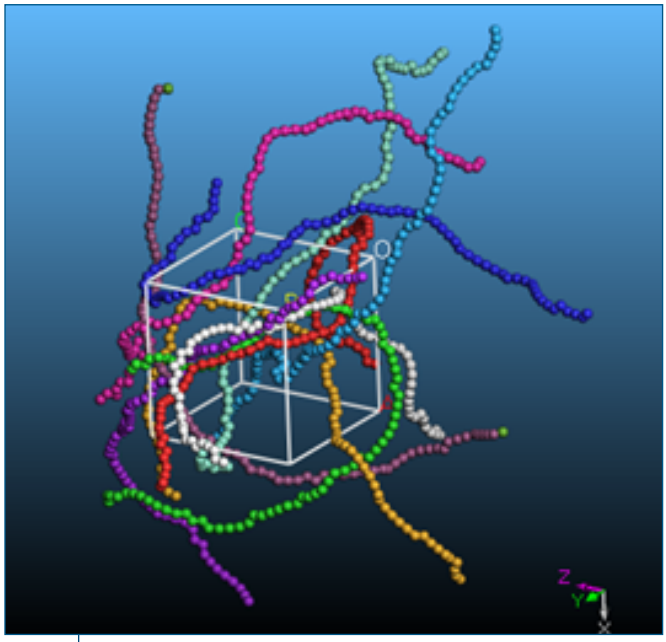


Figure 3: Materials Studio model of packed mesomolecule conformations built according to the forcefield sampling energy.

Bilayer Building

Pipeline Pilot Materials Studio Collection now includes a tool provided in the form of a protocol to build mesoscale membranes. You can find this in the folder dedicated to Coarse Graining tools. The protocol is supplied with ready-made lipid, salt, and solvent molecules typed according to the MS Martini 3 forcefield and can be accessed directly through the Pipeline Pilot Connector. Custom mesomolecules can also be inserted. Lipid mixtures can be defined for membrane sections and used to construct single or double bilayers of arbitrarily complex mixtures with oriented lipid molecules. The protocol will also run equilibration dynamics to provide production-ready configurations. Studies of skin penetration or cell membrane interactions can be greatly accelerated by using this protocol to set up the model systems.

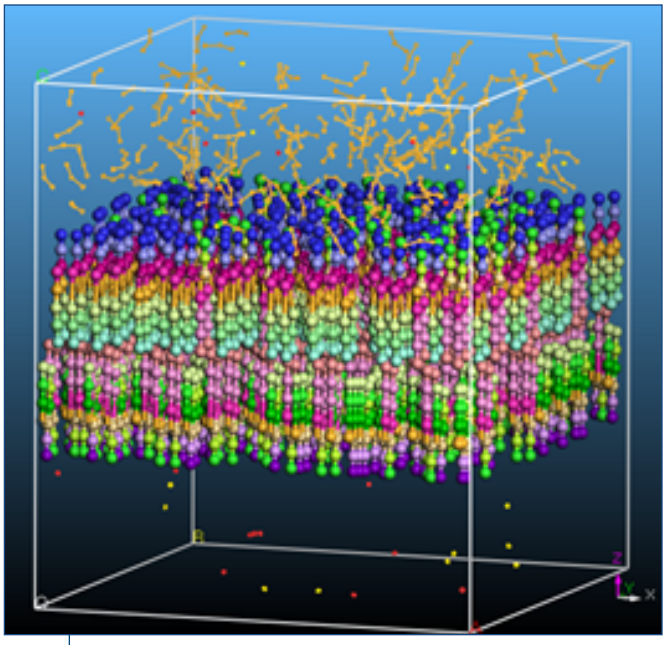


Figure 4: Materials Studio model of packed mesomolecules in a mixed lipid bilayer configuration. The water beads are hidden in this view.

- **New Protocol!** A new protocol Build Mesoscale Membranes using Pipeline Pilot
- **New Component!** A new component creates mesoscale template documents using Pipeline Pilot together with Build Mesostructure from Template component to generate mesostructures.
- **New MaterialsScript!** The Mesostructure Template builder can now be accessed using at Materials Studio scripting.

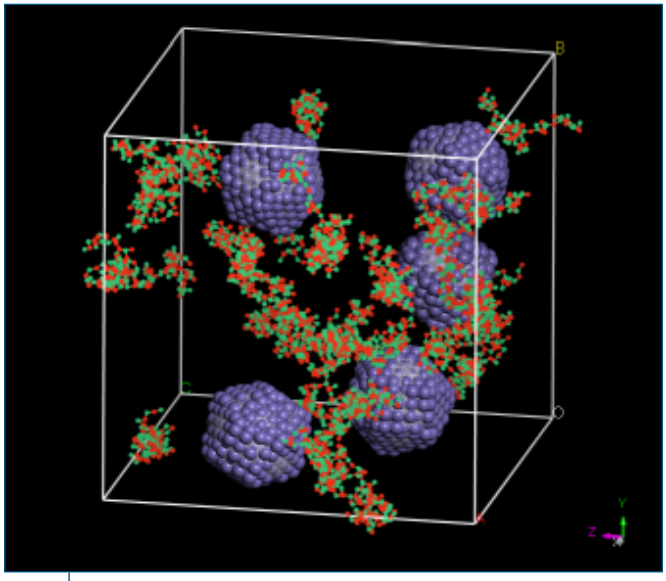


Figure 5: Materials Studio example model of packed mesomolecules in a filled polymer composite material.

Materials Studio 2025 accelerates time to solution for construction of realistic polymeric and lipid membrane systems based on atomistic or coarse-grained models.

Motion Group Support in The Mesoscale Builder

Mesoscale versions of composite materials containing rigid and flexible components can be built using the mesostructure builder by defining rigid units as motion groups. Filled rubbers and battery electrode materials are just two examples that can be studied more easily using this new feature.

MATERIALS STUDIO 2025 FOR MATERIALS SEARCH

A variety of materials databases are increasingly available as a source of molecular models and as materials informatics input. Materials Studio 2025 simplifies the search of disparate data sources by connecting to the Optimade API [7].

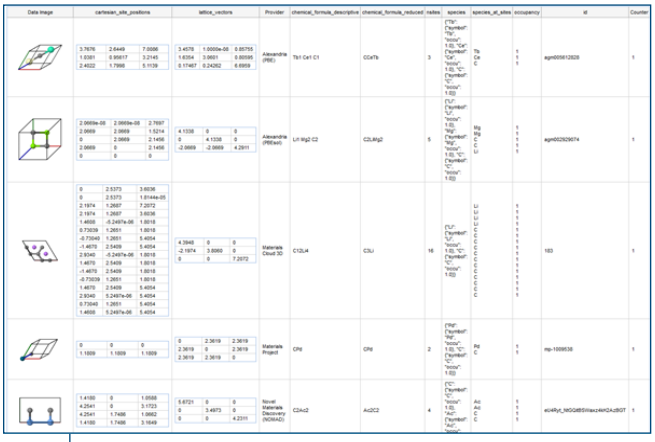


Figure 6: Example results returned from an OPTIMADE search of multiple data sources.

Enhanced Productivity! The new OPTIMADE protocol enables you to:

- Use one query to search multiple databases and return the models as study table of structures and properties
- Construct element based queries or custom queries for more targeted results
- Connect to the large list of pre-configured databases or add URLs to others
- Return models directly to the Materials Studio environment to use in modeling or machine learning workflows

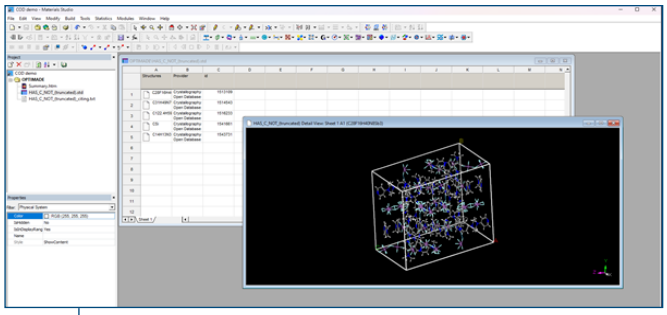


Figure 7: Results of an OPTIMADE search are returned as study tables in Materials Studio to use in modeling or informatics workflows.

MATERIALS STUDIO HIGHLIGHTS BY MODULE

AMORPHOUS CELL

New Performance! Amorphous Cell Construction simulations now have improved performance, in particular for large molecular systems. Constructing atomistic amorphous cell models is now faster and more efficient.

CASTEP

New Parameters! The Grimme D3 dispersion correction is now implemented in CASTEP for some GGA functionals: PBE, PBESOL, RPBE, BLYP. This parameterization covers all elements up to Z=94, so you can use it to study compounds of relevant actinoids.

New Performance! Run CASTEP calculations using GPUs on Linux, providing substantial acceleration of expensive calculations involving nonlocal exchange-correlation functionals.

New Parameters! Run CASTEP using the meta-GGA exchange-correlation functional R2SCAN [5].

New Parameters! Run CASTEP using the Grimme D3 dispersion correction for GGA functionals: PBE, PBESOL, RPBE, BLYP.

New Property! You can now calculate piezoelectric coefficients using the ultra-soft pseudopotential formalism in CASTEP.

New Method! Run CASTEP minimum energy path simulations in conjunction with the FlexTS module to predict reaction pathways.

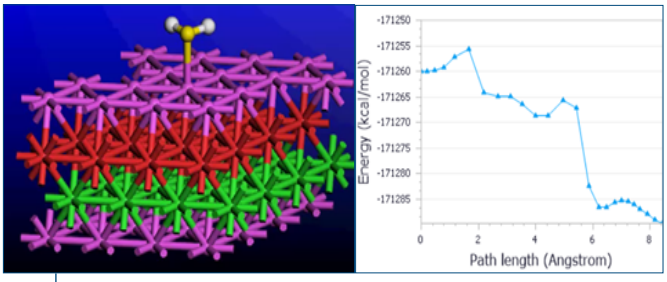


Figure 8: The application of FlexTS with CASTEP as the energy server demonstrating the multistep dissociation of SH2 molecule on aluminium. (a) The starting configuration (b) the minimum energy path provided by FlexTS.

COMPASS

New Parameters! You can now more-accurately model systems containing barium ions, titanates, and N-O bonds in aromatic systems.

New Parameters! The bond stretch and van der Waals parameters for molecular hydrogen (H2) in COMPASSIII have been updated to improve diffusional properties.

New Parameters! Improved parameters for modelling phosphoric acid.

New Parameters! New forcefield type p3 in COMPASSIII provides support for phosphorus trihalides, such as PF3.

DFTB+

New Spectra! You can now use the DFTB+ frequency property option to generate predicted vibrational spectra to help you to understand molecular properties and compare simulations with experimental results.

New Performance! The DFTB+ solver now takes full advantage of the DFTB+ API resulting in a significant performance improvement for small systems.

FORCITE

New Performance! Building on improvements over the last several releases the performance on GPUs has been increased further.

New Peformance! Run Forcite molecular dynamics with enhanced performance on GPUs using GPU accelerated group sum method for van der Waals and electrostatic interactions.

New Property! Calculations of radial distribution functions have improved performance, especially for systems with many atoms or beads.

GULP

Upgraded Solver! The GULP solver has been updated to academic version 6.3.

MESOCITE

New Tasks! Mesocite now includes a new Builder tool to help you to construct mesoscale amorphous cells using mesomolecules and Mesocite forcefields through new Construction, Packing, and Confined Layer tasks.

New Performance! The Mesocite solver benefits from GPU performance efficiencies to improve productivity.

ONETEP

Upgraded Solver! The ONETEP solver has been updated to academic version 7.1.

VISUALIZER

Updates to the Materials Studio Visualizer include:

- The mesostructure builder now supports motion groups to allow packing of templates with both rigid and flexible molecules.
- When you build mesoscale molecules, you can now choose to randomize the conformation of the molecules
- Calculation of bonds for periodic nanotubes now more accurately generates bond orders.
- Two new scripts in the Materials Studio Scripts menu enable you to calculate ion clustering in trajectories with a bespoke Cluster Population Analyses method and to visualize the outcome using of heat maps using generated plots.

ENHANCEMENTS TO PIPELINE PILOT PROTOCOLS

The Pipeline Pilot Protocols Connector dialog provides access to enhancements available in the Pipeline Pilot Materials Studio Collection, enabling you to

- Calculate optical properties using TD-DFT formalism
- Build a Mesoscale Membrane model or Mesoscale Template system
- Run a Calculate Glass Transition Temperature protocol or Calculate Yield Stress and Critical Distortional Strain protocols using study table input
- Query the databases available via OPTIMADE API [6][7]
- Use a new component for Crystal Graph (Morphology)
- Uses a new protocol to Calculate Morphology using a Crystal Graph

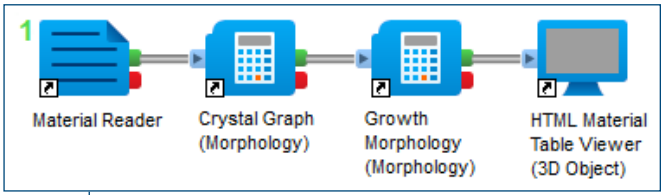


Figure 9: Image showing the use of the new crystal graph component in the new Calculate Morphology using a Crystal Graph protocol supplied in Pipeline Pilot Materials Studio Collection 2025.

TUTORIALS

The following new tutorials have been added:

- Effective screening medium (ESM) in DMol3.
- Building Mesoscale Amorphous Cell Using Mesocite Builder.

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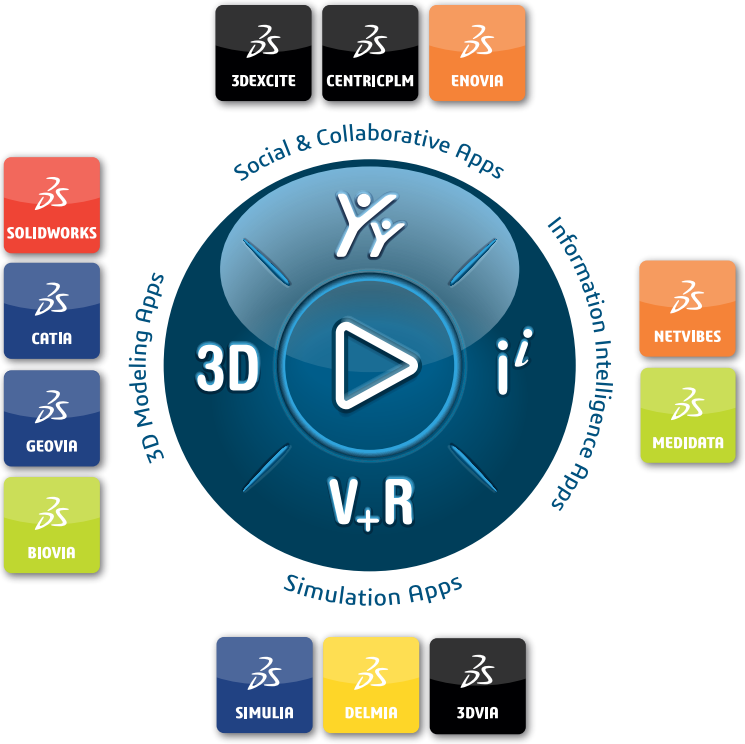

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