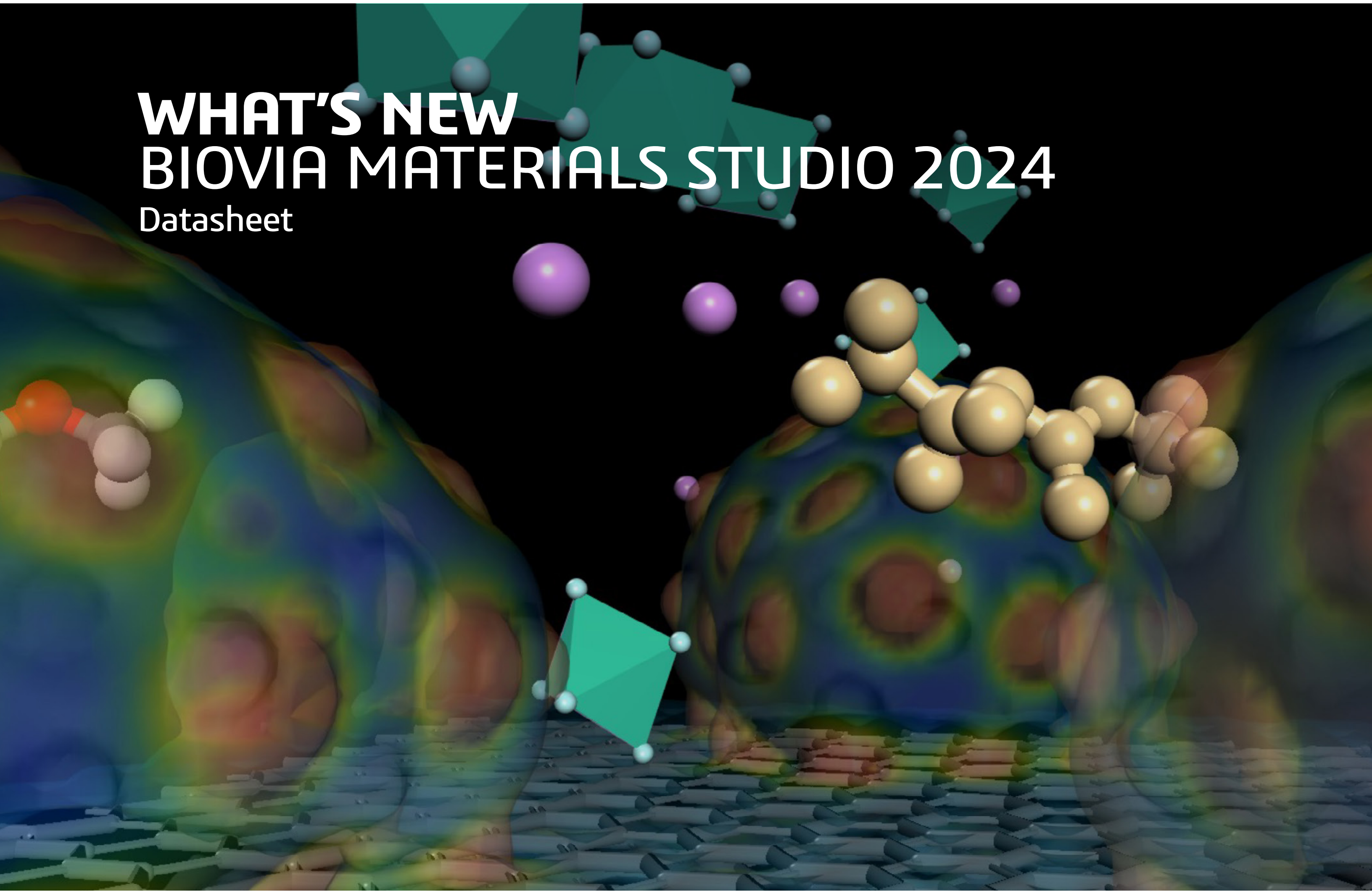
WHAT'S NEW
BIOVIA MATERIALS STUDIO 2024
Datasheet



BIOVIA Materials Studio 2024 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 the material's molecular or crystal structure and its properties. Scientists using BIOVIA Materials Studio 2024 have access to an extensive suite of world-class solvers and parameter sets operating from quantum to microscales.

This release contains enhancements across the full range of scales, from atoms to microscales, and, in particular, introduces a new method for simulating granular materials, new treatments of electrochemistry at surfaces in the presence of electric fields, and tools for running reactive kinetic Monte Carlo Molecular Dynamics.
With these new advances, and combined with enhanced support for GPU processors, you can simulate more material properties more accurately and more quickly than ever before.

Key Values:

- Accurately simulate complex reactive systems and surface reactions for enhanced scientific insights in the study of catalysts, battery interfaces, and more.
- Integrate metal alloy microstructure development for optimized additive manufacturing workflows.
- Thoroughly study particle grain-scale structure formation and simulate structural changes during manufacturing.

BIOVIA MATERIALS STUDIO 2024 FOR ELECTROCHEMISTRY

Materials Studio provides a comprehensive solution for studying chemical reactions through the application of quantum mechanical solvers (CASTEP, DMol3, DFTB+ ONETEP, and VAMP), chemical transition state searching (FlexTS), and reaction kinetics predictions (Cantera and Kinetix). Materials Studio 2024 adds further capabilities in this area, enabling the simulation of the long-time evolution of complex reactive mixtures and predicting chemical reactions at surfaces in the presence of electric fields.

REACTIVE MOLECULAR DYNAMICS

Kinetic Monte Carlo–molecular dynamics (kMC-MD) is a method for simulating reactive liquids using otherwise non-reactive force-fields and classical simulations to evolve the system. The ReactionFinder kMC-MD feature was integrated into Forcite to provide a generalized approach to simulating reactive systems, allowing observation of their evolution over much longer timescales than achievable with pure quantum mechanical methods (Abbott, 2022). This release introduces a protocol for constructing reaction mechanisms of arbitrary complexity, defining the input for ReactionFinder. It includes a comprehensive user interface for setting parameters in ReactionFinder and tools for analyzing the composition of the resulting product box.

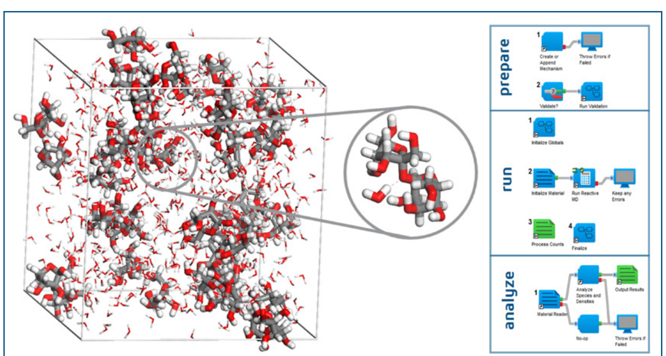


Figure 1: Example application for the 'Run Monte Carlo Reactive Molecular Dynamics Simulation' protocol showing liquid electrolyte mixture typical of lithium ion batteries

New Usability! The latest Materials Studio Collection protocols enable the preparation and execution of reactive Monte Carlo Molecular Dynamics simulations with specific provisions for electrochemistry. You can define individual reactions using graphical tools in Materials Studio, ensuring their suitability within ReactionFinder to prevent runtime errors or unexpected reactions. The identification of reactions also automatically considers molecular symmetries for performance efficiency.

New Analysis! A new protocol allows the analysis of ReactionFinder output, creating species distribution counts with options to plot concentration profiles, download as a .csv file, and color code species in the models for visual identification assistance.

Build, simulate, analyse complex reactive systems to unlock new scientific insights. With reactive molecular dynamics you can study a variety of processes such as polymerization, resin curing, degradation and liquid chemistry including how complex structures such as battery solid electrolyte interphases evolve.

REACTIONS AT SURFACES

Materials Studio 2024 introduces new features to DMol3, ONETEP, and GULP, enabling reactions at surfaces while considering the presence of electric fields. Although these features are general additions to each module, they present an opportunity to investigate the interfaces of battery electrodes with liquid electrolytes, where complex chemical reactions occur in the presence of electric fields.

New Method! The Effective Screening Medium (ESM) option in DMol3 has been introduced. This option replaces the periodic boundary condition along the z-direction with a screening medium, such as a vacuum or metal, at the cell boundary. The Effective Screening Medium (Otani, 2006) applies a non-periodic boundary condition for the electrostatic field along the surface normal direction (z-direction) of a slab model, eliminating the need for a large vacuum region in the z-direction. The option to add a metallic medium to the model allows for calculations with charged slab systems, simulating gate effects as well as biased systems. The metal boundary mirrors any charges in the system, and DMol3 fixes the potential of the metal boundary at 0 eV.

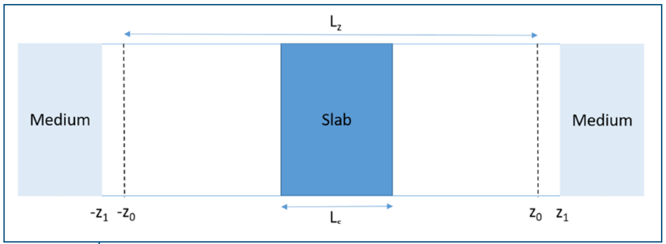


Figure 2: Effective Screening Medium (Otani, 2006) applies a non-periodic boundary condition for the electrostatic solution along the surface normal direction (z-direction) of a slab model. The mediums are either vacuum (ε=1) or metal (ε=∞).

New Parameters! You can now utilize the latest GULP ReaxFF library, ReaxFF SEI2021 (Liu, 2021), for modeling the surface-electrolyte interphase.

New Options! Additionally, you can calculate properties for variable charge models, including charge derivatives for electric fields. This enhancement enables GULP ReaxFF calculations with electric fields.

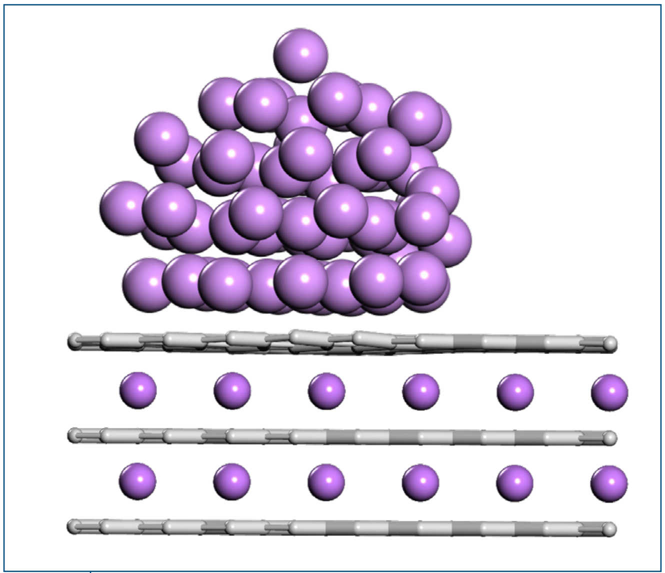


Figure 3: Model of a lithium nanocluster on a lithiated graphite electrode material. ONETEP has been used to study the potential of zero nucleation energy in various scenarios, supporting hypothesis about the conditions in which lithium clustering and subsequent dendrite growth may occur. (Bhandari, 2022)

New Method! The grand-canonical ensemble is now implemented in ONETEP for simulating systems with a variable number of electrons and a fixed external potential. This functionality is especially relevant for electrochemical studies of electrode-electrolyte interfaces. For instance, Bhandari (2022) investigated the conditions triggering lithium dendrite growth in lithium-ion batteries. The study involved building surface models of lithiated and unlithiated graphite topped with lithium clusters and using a continuum solvent to represent a typical liquid electrolyte medium

Simulate reactions at surfaces enabling detailed study of catalyst surface reactions and battery electrode interfaces

BIOVIA MATERIALS STUDIO 2024 FOR MICROSTRUCTURE DEVELOPMENT

Controlling the processing of materials is often critical to optimizing their performance, requiring consideration of physics at much larger length and time scales than the molecular level. An example of this is the grain microstructure in metal materials, where specific methods are needed to predict the size, shape, and orientation of grains. One such method is the phase field method, which is included in the Pipeline Pilot Materials Studio Collection 2024.

METAL ALLOY MICROSTRUCTURE

BIOVIA Materials Studio offers a comprehensive solution for the development of metals, covering first principles phase diagram generation to the simulation of microstructures. The PhaseField module enables users to define component phases, set up grains, input thermodynamic and kinetic parameters, and specify temperature and pressure conditions through a user-friendly interface in the Pipeline Pilot Connector. This facilitates detailed studies of phase transitions in multicomponent metal alloys. In Materials Studio 2024, new features enhance the efficiency of running PhaseField simulations.

Increased Performance! The PhaseField protocols now feature an option for running simulations with adaptive time stepping. The phase field code estimates the required time step for accurate calculations and continuously updates the step size as the system evolves.

Increased Productivity! The Solidification and Grain Growth PhaseField protocols now support restarts using the final field setup from a previous simulation.

Multiscale Advantage! Connections between PhaseField results and Abaqus finite element simulations, along with the MicroMechanics plugin, have been enhanced in Materials Studio 2024. The new features include:

- An option to remesh Abaqus input files with a coarser mesh, ensuring that the microstructure imported into Abaqus is better suited for finite element analysis.
- The ability to use GRAIN set definitions to specify grains.
- The capability to define faces of the cell, supporting the configuration of periodic boundary conditions.

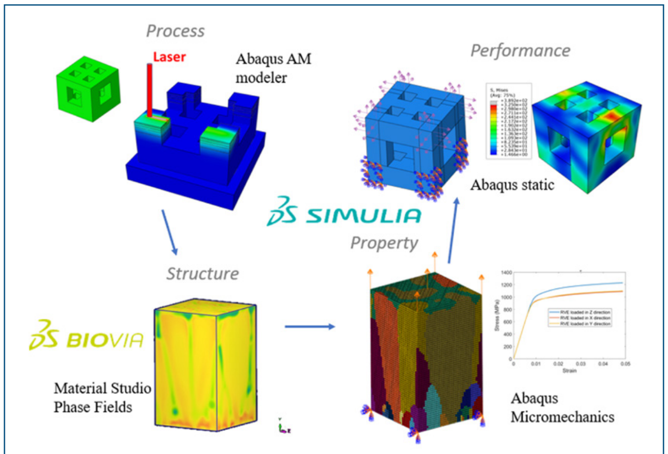


Figure 4: Schematic of the multiscale approach to simulation of additive manufacturing starting with SIMULIA Abaqus models of laser scintillation process and incorporating BIOVIA PhaseField simulation of the grain microstructure (Reig Buades, 2023).

Integrate metal alloy microstructure development into workflows providing optimization of metal additive manufacturing processes.

GRANULAR DYNAMICS

The processing of granular materials is crucial in various industries, such as pharmaceutical tableting and the compaction of aggregates (e.g., concretes). Another pertinent example is the manufacture of battery electrodes from electrode slurry mixtures. In these cases, the arrangement of active particles after processing governs the conductive pathways through the composite material. These pathways directly impact charging and discharging profiles, emphasizing the importance of controlling particle packing to optimize these pathways.

Granules in such applications are often large enough that, unlike molecular simulations, thermal forces no longer dominate the motion. Instead, forces are determined by contact/collision models that incorporate macroscopic phenomena such as friction and gravity. In response to these material processing challenges, Materials Studio 2024 introduces a new granular dynamics task to the Mesocite module.

New Method! Now, you can utilize the Granular Dynamics task in Mesocite to simulate the motion of particles with negligible thermal velocity, predicting the arrangement of mixed particle systems.

New Tutorial! A tutorial on the preparation of granular material has been introduced. This tutorial demonstrates the practical application of the Granular Dynamics task in Mesocite.

New Scripts! Additionally, new scripts have been provided to support the construction of granular material models and simulate solvent evaporation and calendaring.

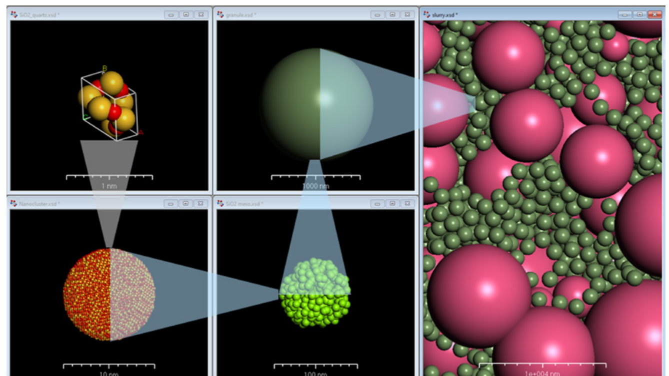


Figure 5: Scales accessed in granular dynamics are significantly larger than molecular or coarse-grained models.

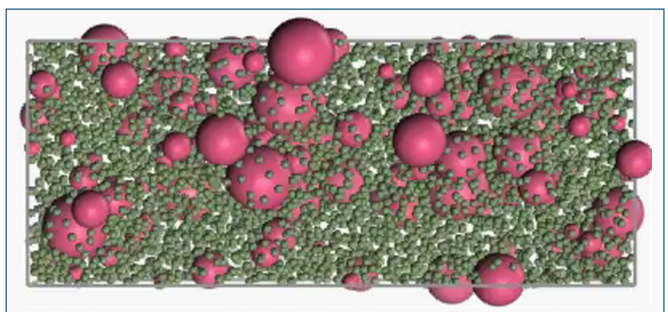


Figure 6: Simulation model of mixed granular materials representing battery electrode slurry

Study the formation of structures at the scale of particle grains and simulate how those structures change during manufacturing steps.

MATERIALS STUDIO 2024 HIGHLIGHTS BY MODULE

DMOL3

New Method! The Effective Screening Medium (ESM) option in DMol3 is now available. This option replaces the periodic boundary condition along the z-direction with a screening medium, such as a vacuum or metal, at the cell boundary. The metal boundary mirrors any charges in the system, enabling the analysis of charged systems. DMol3 fixes the potential of the metal boundary at 0 eV. Additionally, for metal-metal systems, you can introduce an electric field to apply a bias between the metal surfaces.

CASTEP

New parameters! A DFT-D4 semi-empirical dispersion correction, which is faster than the many-body dispersion correction (MBD*), produces accurate structures and energies for molecular crystals and systems with important van der Waals contributions to the interactions. (Caldeweyher, 2020)

CCDC

Materials Studio integration with the CCDC tools supports CSD 2023 installation.

COMPASS

New Parameters! New COMPASS III force-field charges, specifically the bond increments for the n4+ and h1+ forcefield types for ammonium (NH4+) provide improved density predictions.

DFTB+

New Systems! DFTB+ now uses version 22.2, which includes the ELPA eigensolver. The ELPA solver supports GPU acceleration, offering a significant additional performance gain for large systems. GPU acceleration also supports the use of multiple GPUs, scaling effectively on massively parallel supercomputers and exhibiting great efficiency for smaller systems. This opens up new possibilities for large-scale simulations, such as nanoparticles and complex battery materials.

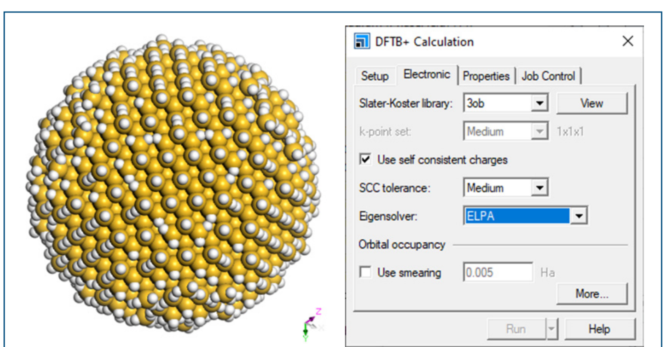


Figure 7: A silicon nanoparticle with 15991 orbitals. Large scale multi-GPU DFTB+ calculations are now available in Materials Studio 2024.

FORCITE

New Method! Forcite now has a new barostat, Anisotropic. This allows you to vary the three cell lengths independently (or to remain fixed) and to apply a different stress to each face of the cell. You can model uniaxial extension and carry out equilibration of interface models more easily.

New Performance! A series of enhancements to GPU performance, including the capability to run with electric fields through GPU compute resources, delivers a significant increase in overall performance. Furthermore, Forcite calculations can now be executed on an expanded range of NVIDIA GPU cards (refer to the System Requirements document for details).

New Property! The Dipole Autocorrelation Function analysis tool is available to calculate the running average of the static dielectric permittivity of the trajectory, as well as the permittivity storage and loss spectrum. Due to the long correlation times involved in dipole autocorrelation function calculations, additional tools are provided to generate and analyze multiple sampling trajectories. This enables the convergence of predictions and facilitates fitting to functions based on Debye relaxation times.

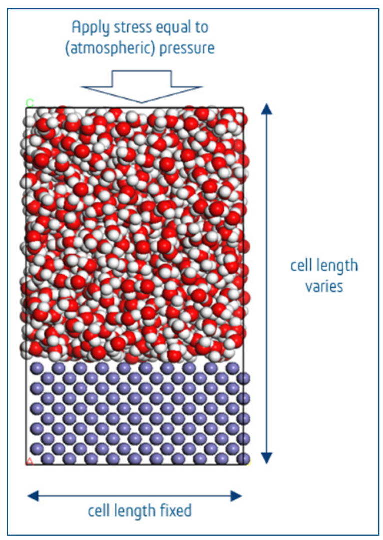


Figure 8: An anisotropic barostat option available in Forcite and Mesocite allows for easier equilibration of liquids on surfaces

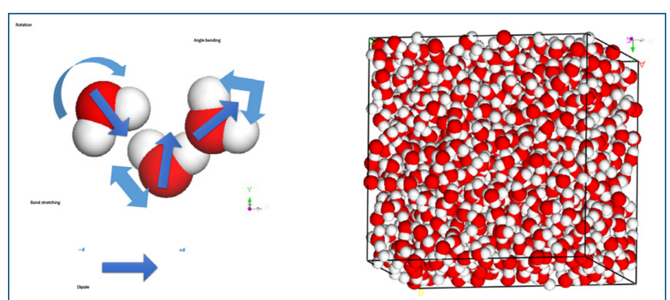


Figure 9: Image of dielectric loss function for water. In Materials Studio 2024 you can calculate the static dielectric permittivity and the permittivity storage and loss spectrum as a new option on the dipole autocorrelation analysis dialog.

GULP

The GULP solver has been updated to academic version 6.2 and provides the following feature updates

- A new GULP ReaxFF library for modeling the surface-electrolyte interphase. This library, ReaxFF SEI2021 (Liu, 2021)
- Calculation of properties for variable charge models with charge derivatives including those for electric fields; enabling ReaxFF calculations with electric fields.
- Access to two new force-field libraries AA-CLP (Gavezzotti, 2011) and Nitrates (Fantauzzo, 2022)
- Calculation of charges for s and p block elements using extended Huckel theory, in particular, to support the AA-CLP force-field
- ReaxFF calculations that include analytic second derivatives and phonons, so that you can evaluate full phonon dispersion and phonon density of states

MESOCITE

Materials Studio 2024 introduces a multitude of updates to the Mesocite module for coarse-grained simulations, including:

New Tasks! Mesocite now supports Anneal, Quench Dynamics, Confined Shear, Solvation Free Energy, Cohesive Energy Density, and Mechanical Properties calculations for mesostructures.

New Method! The latest addition is the Granular Dynamics task, allowing the simulation of particle motion with negligible thermal velocity.

New Method! Mesocite introduces a new Anisotropic barostat, enabling the independent variation of three cell lengths or keeping them fixed, and the application of different stresses to each face of the cell.

New Performance! Mesocite calculations are significantly faster when run using GPUs. Additionally, an extended range of NVIDIA GPU cards is now supported (refer to the system requirements document for details).

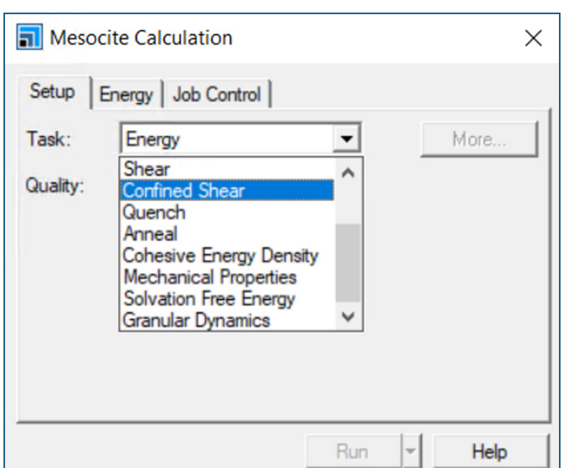


Figure 10: Mesocite user interface showing new tasks available in Materials Studio 2024.

ONETEP

New Method! The ONETEP solver code has been upgraded to the academic version 6.1.45, now featuring a grand-canonical ensemble for simulations of systems with a variable number of electrons and a fixed external potential.

VISUALIZER

Updates to the Materials Studio Visualizer include:

- An option to specify exclusion rules for valence terms that are missing from force-fields.
- New matching criteria for bonds in the Find Patterns tool.
- Addition of a PDF version of the introductory content of the Materials Studio online help.

ENHANCEMENTS TO MATERIALSSCRIPT

Materials Studio 2024 offers several new features, allowing you to:

- Create bead types from MaterialsScript for use in coarse-grained simulation workflows.
- Script all Forcite and Mesocite tasks available through the Visualizer user interface
- Select close contact and hydrogen bond objects locally making selection much more efficient
- Find close contacts between both beads and atoms

Additionally, you can now launch MaterialsScript jobs directly from the Detail View of a structure in a study table. This functionality works seamlessly with both direct MaterialsScript jobs and those launched from custom User Menu commands.

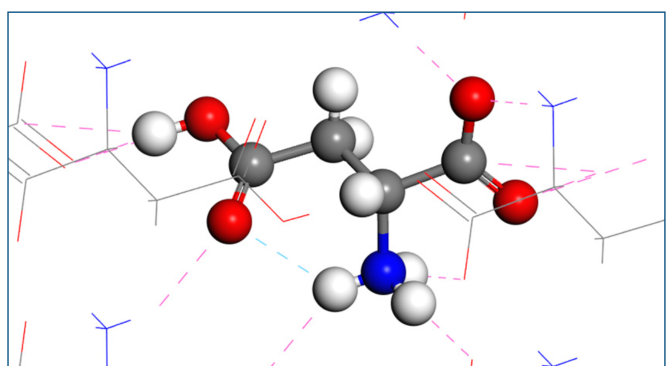


Figure 11: Close contacts selection is more efficient in Materials Studio 2024

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

- Prepare, run, and analyze reactive Monte Carlo Molecular Dynamics simulations with specific provisions for electrochemistry.
- Generate Materials Studio XSD files from SMILES strings or the chemical names of molecules.
- Run PhaseField simulations using adaptive time stepping. The phase field code now estimates the time step needed for an accurate calculation and continuously updates the step size as the system evolves.
- Restart Solidification and Grain Growth PhaseField simulations using the final field setup from a previous simulation.
- Use a wider set of exchange-correlation functionals for calculating Semiconductor Band Offsets and Equations of State for Solids
- Calculate thermal conductivity in an amorphous system or periodic cell through the Pipeline Pilot Connector using Reverse Non-Equilibrium Molecular Dynamics method (Previously provided as a prototype)

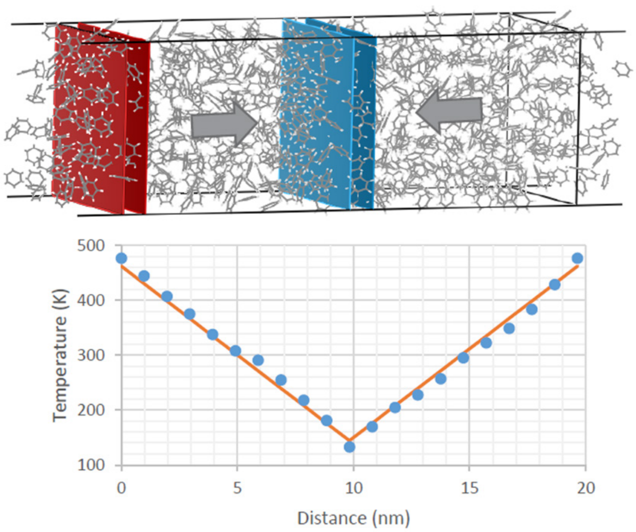


Figure 12: Example of Reverse Non-Equilibrium Molecular Dynamics used to measure thermal conductivity now available through the Pipeline Pilot Connector in Materials Studio 2024

TUTORIALS

The following new tutorials have been added:

- **Polymer Coarse Graining with Martini 3 Tools:** Demonstrates how to generate templates for bead mapping, use templates with the MS Martini 3 Coarse Grainer, and customize the MS Martini 3 force-field for a given polymer structure.
- **Preparation of a Granular Material:** Demonstrates the use of the Granular Dynamics task in Mesocite.

The following new tutorials have been updated:

- **Calculating the Miscibility of Two Polymers:** Includes an improved workflow for the calculation of polymer properties.
- **Cross-linking polymers using Pipeline Pilot:** Provides additional information about other reaction types during creation of a polymer network.

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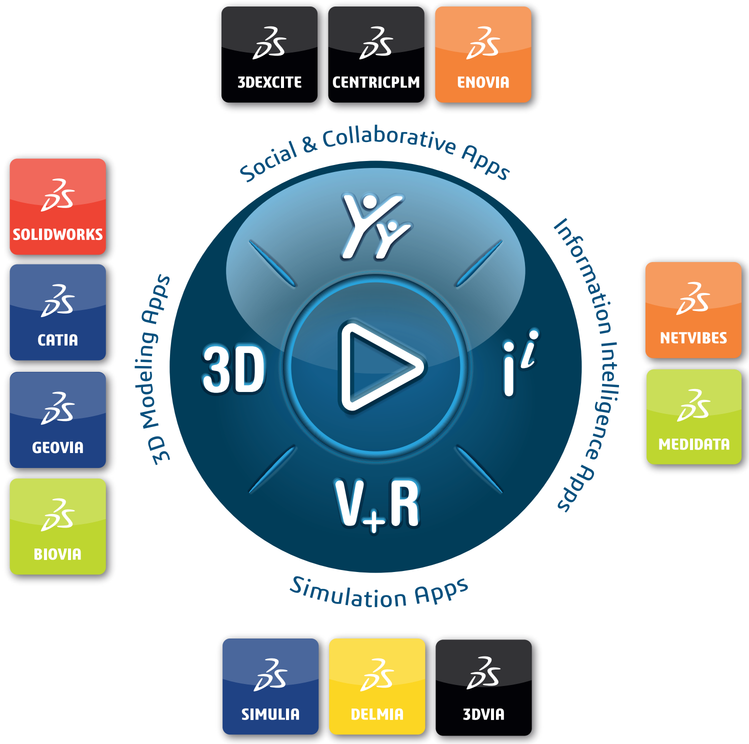

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DS-10038-0124