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WHAT'S NEW IN BIOVIA MATERIALS STUDIO 2021

Datasheet

BIOVIA Materials Studio 2021 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 arising at multiple scales.

Scientists using BIOVIA Materials Studio 2021 have access to an extensive suite of preeminent solvers and parameter sets operating from atoms to microscale, and this release adds two new methods: 1) for robust transition state searching and 2) for phase field modeling of hard material microstructure. This release also features the introduction of GPU processor support to Materials Studio, significantly accelerating classical simulations.

With BIOIVA Materials Studio 2021, scientists can simulate more material properties, more accurately and more efficiently than ever before.

DASSAULT SYSTEMES

NEW MODULE!

BIOVIA MATERIALS STUDIO FlexTS END-TO-END REACTION KINETICS

Density functional theory allows scientists to use changes in electronic structure to predict individual chemical reactions to a high degree of accuracy. However, the goal of a chemical engineer is to model reaction mechanisms involving potentially complex conflagration of interdependent reactions—the chemical reaction kinetics. The primary bridge to reaction kinetics is 1) the identification of a transition state for each reaction corresponding to the saddle points on the energy landscape between reactant and product, and 2) the size of the activation barrier.

Based on code developed at the University of Cambridge [Munro et al. (1999), Kumeda et al. (2001), Trygubenko et al. (2004), Carr et al., (2005) and Wales et al. (2012)], BIOVIA Materials Studio FlexTS introduces robust reaction pathway calculations including minimum energy pathways, transition states and identification of multi-step reactions. BIOVIA Materials Studio FlexTS employs a hierarchy of methods to identify the minimum energy path and subsequently calculate the transition states and location of the minima corresponding to each transition state. The FlexTS Minimum Energy Path methods are available as tasks from either BIOVIA Materials Studio DMol^3 or from BIOVIA Materials Studio DFTB$^+$. Access to DMol^3 or DFTB$^+$ modules is required in order to compute the energy landscape explored by FlexTS. There are three available run modes:

- **Full Path**: a double-ended task that finds one or more transition states required to connect reactant and product.
- **Nudged Elastic Band**: a double-ended task that runs a Nudged Elastic Band calculation for a given number of images and iterations or to a convergence threshold provided by the user. This task is useful for studying very small barriers or barrierless reactions.
- **TS Path**: a single-ended transition state search that starts from the guess for a transition state and refines it. Then the tool calculates the reactant and product minima corresponding to the transition state.

A new tutorial exploring the functions of FlexTS is available from the Materials Studio Online Help to guide you through the new features.

With knowledge of transition states obtained from FlexTS, the reaction kinetics task in Dmol^3 can provide rate coefficients that are in turn inputs for BIOVIA Materials Studio Cantera and BIOVIA Materials Studio KINETIX modules. With BIOVIA Materials Studio 2021, chemists and chemical engineers have a powerful, robust and flexible suite of methods to bridge from quantum mechanics to chemical reaction kinetics.

- Numerically stable and easy-to-use transition state searching
- Multiple options for reaction pathways, TS refinements, low barriers
- Study reactions using multiple tools (DMol^3, DFTB$^+$, FlexTS, Reaction Preview, Reaction Kinetics, Kinetix, Cantera) within the Materials Studio environment

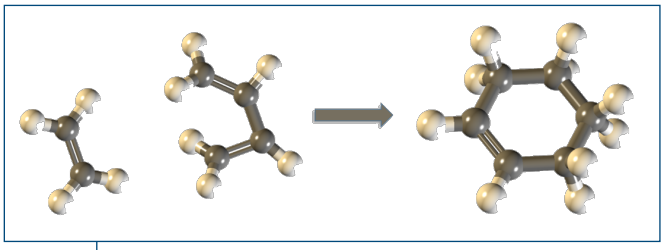

Figure 1: Images of example chemical reaction treated by FlexTS: Diels-Alder ethene (C_2H_4) reaction with butadiene (C_4H_6) .

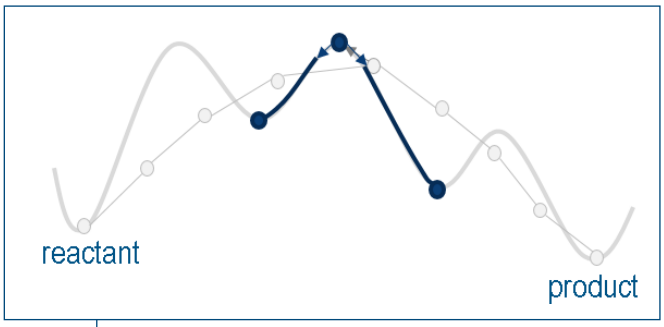

Figure 2: Diagram of a typical path cycle of a transition state search.

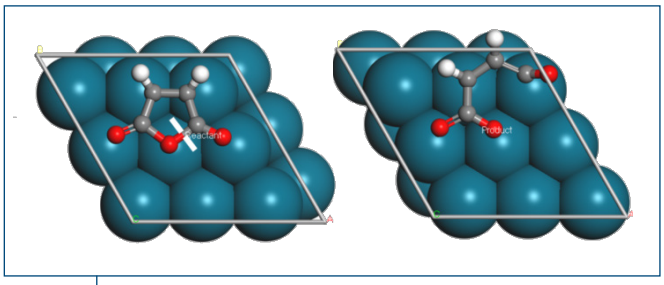

Figure 3: Images of an example chemical reaction on a surface treated by FlexTS: ring opening on a platinum surface.

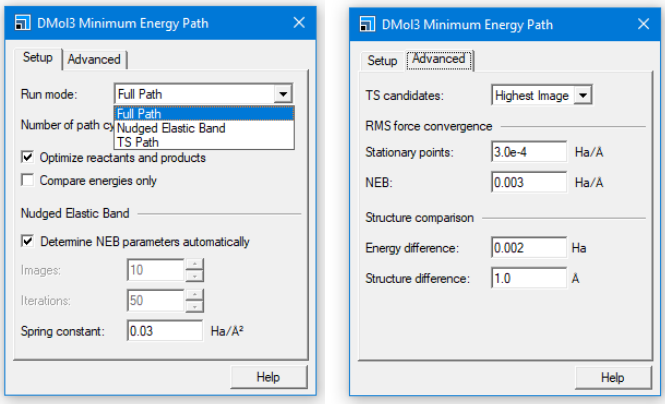

Figure 4: Dialogs showing new tasks available in DMol^3 for running FlexTS tasks.

NEW MODULE!

BIOVIA MATERIALS STUDIO PHASEFIELD END-TO-END METAL ALLOY DESIGN

Understanding how the microstructure of hard materials such as superalloys changes as a function of the thermal and mechanical history is extremely important for determining the performance of a manufactured part. Internal stresses frozen in during manufacturing can lead to deformation of materials during machining or in use. These can occur on the length scales of the individual metal grains and can culminate in part failures.

Through detailed understanding of the grain composition and evolution during processing, metallurgists and materials scientists work to optimise the material composition and processing conditions with a view to producing material that meets engineering specifications within the constraints of the manufacturing process. Traditionally, many physical tests and material characterization experiments are required to achieve a thorough understanding of the material and eventual certification. Predictions of the response of the material microstructure to changes in composition or solidification conditions through simulation can significantly accelerate these investigations.

Phase-field simulation [Steinbach (2009), (2013)] is a long established method—focussed on microstructure evolution at the mesoscale—for understanding solidification, phase transformations, dendrite growth, coarsening and grain growth in solid-state materials. To make microstructural predictions, BIOVIA Materials Studio PhaseField employs the OpenPhase_Core solver [OpenPhase Solutions GmbH], which is a mature and highly validated implementation of the phase-field method. Phase-field represents materials as distributions of grains at the mesoscale, where each grain relates to the composition and orientation of crystal phases. By using equations that describe the thermodynamic and kinetic character of the phases, we can determine the evolution of the phases. We can then measure or simulate a number of physical parameters that embody these characteristics.

Pipeline Pilot Materials Studio Collection protocols provide access to the phase-field method and are available through the Pipeline Pilot Connector in Materials Studio 2021. Two new tutorials in the Materials Studio Online Help provide guidance in using these protocols. BIOVIA Materials Studio PhaseField provides a convenient way to define the component phases, grain set up, thermodynamic and kinetic input and temperature/pressure conditions, through a simple-to-use interface.

ADDITIVE MANUFACTURING

One important application of the phase-field method is metal additive manufacturing. We can use BIOVIA Materials Studio PhaseField to understand dependence of microstructure on the print conditions during powder bed fusion additive manufacturing in which individual layers of metal alloy powder are melted by laser or electron beam and then cool. Microstructural simulations provide an opportunity to design the material composition and manufacturing conditions together, in order to meet the required specifications of the printed part.

The microstructures predicted by BIOVIA Materials Studio PhaseField provide a direct view into the grain size and distribution of phases. We can also use them to provide homogenized materials properties for the modelled representative volume element (RVE). PhaseField produces SIMULIA Abaqus-ready versions of the RVE to streamline this activity.

With BIOVIA Materials Studio 2021, materials scientists and metallurgists can use the BIOVIA Materials Studio PhaseField to bridge from the first principles prediction of metal alloy thermodynamics at atomistic scales (provided by application of quantum mechanics and cluster expansion methods that are already available) through to the macroscopic world of metal casting and additive manufacturing. With end-to-end simulation of these materials now incorporating the impact processing conditions on microstructure, we can significantly accelerate the development and certification of metal alloys for part manufacture.

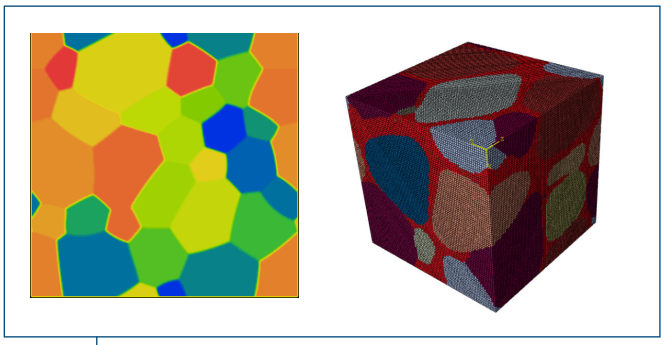

Figure 5: Two example microstructure outputs from BIOVIA Materials Studio PhaseField simulation showing the boundaries between grains. The first is a 2D field density view inside Materials Studio 2021 and the second shows a voxel representation inside SIMULIA Abaqus software.

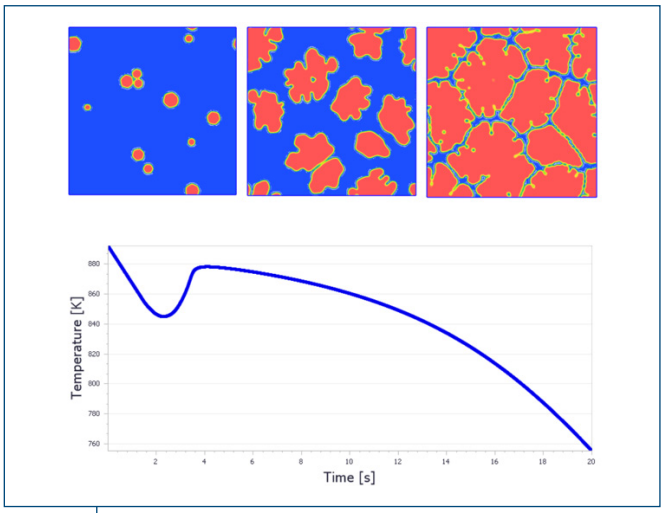

Figure 6: Output from a BIOVIA Materials Studio PhaseField simulation showing nucleation and growth of an aluminium-magnesium alloy during cooling.

MATERIALS STUDIO MODULE ENHANCEMENTS

CLASSICAL SIMULATION ENHANCED PERFORMANCE! MORE MATERIALS!

Materials Studio 2021 brings the highly functional classical molecular dynamics methods in Forcite and Mesocite solvers to NVIDIA GPU processors. We can now run molecular and coarse-grained dynamics on a GPU providing more than an order of magnitude speed-up over traditional CPU performance onWindows and Linux.

Additionally, new COMPASS III parameters for battery materials extend the range of materials that we can simulate with confidence using Materials Studio.

Forcite

New Performance! All supported queuing systems can now request the use of GPU in Forcite calculations.

New Function! Urey-Bradley interactions and CHARMM inversions in Materials Studio forcefields.

New Function! Van der Waals functional form LJ_12_6_14 for Materials Studio forcefields providing the opportunity to specify different R0 and D0 values for 1-4 interactions.

New Parameters! An augmented version of the cvff forcefield, cvff_aug, can be now imported providing for construction of amorphous glass models.

COMPASS

New Parameters! COMPASSIII has been extended to support boron compounds relevant to lithium-ion batteries, such as bis(oxalate)borate, difluoro(oxalate)borate and pyridine boron trifluoride.

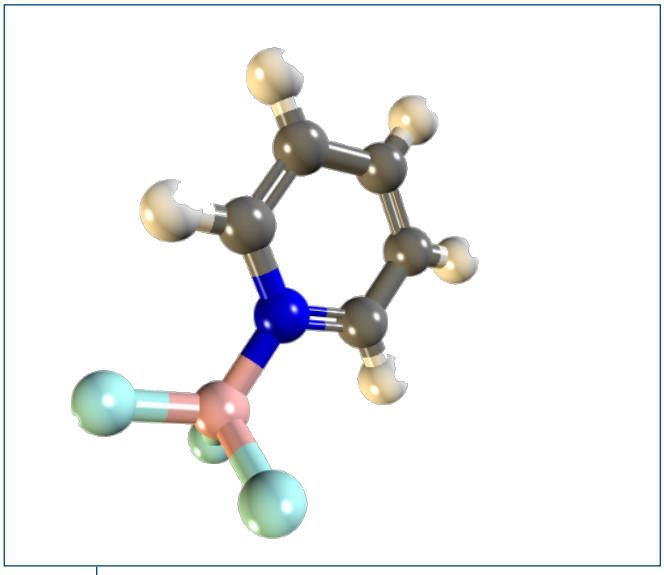

Figure 7: Pyridine boron trifluoride molecule refitted for COMPASS III.

GULP

Upgraded Solver! We have upgraded GULP to version 6.0.

New Method! GULP now supports rigid molecules for geometry optimization and subsequent property and phonon calculations for bulk systems of any periodicity.

New Parameters! A new ReaxFF library, "ReaxFF SEI," is now included. It is based on Hossain et al. (2020) and aims at description of Li-battery electrolytes and solid-electrolyte interphase.

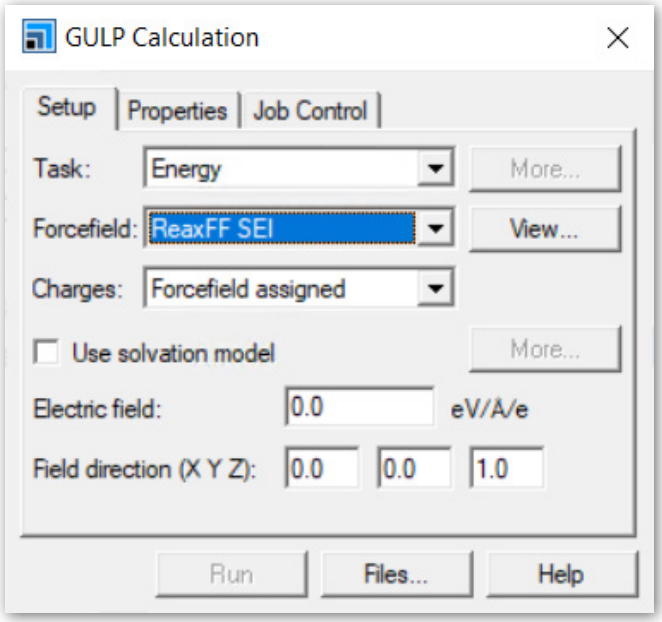

Figure 8: Dialog showing the new GULP force-field option for solid electrolyte interphase reactions.

QUANTUM MECHANICAL SIMULATIONS

New features available in CASTEP, DMol³ and ONETEP extend the available options and material property predictions.

CASTEP

New Property! The fracture toughness estimate calculated using an empirical model of Niu et al. (2019) for brittle materials is now included in the results of elastic coefficients calculations.

New Method! Solvation energy calculations for isolated molecules.

New Materials! Calculation of the tensor of second harmonic generation coefficients for simulation of nonlinear optical materials.

New Property! Berry phase calculation of spontaneous polarization.

New Options! We have extended the spin-orbit coupling implementation in CASTEP to include:

- On-the-fly-generated, norm-conserving pseudopotentials
- Calculation of optical properties
- Calculations using nonlocal exchange-correlation functionals
- A mechanism to set up non-collinear spin configurations in the Materials Visualizer

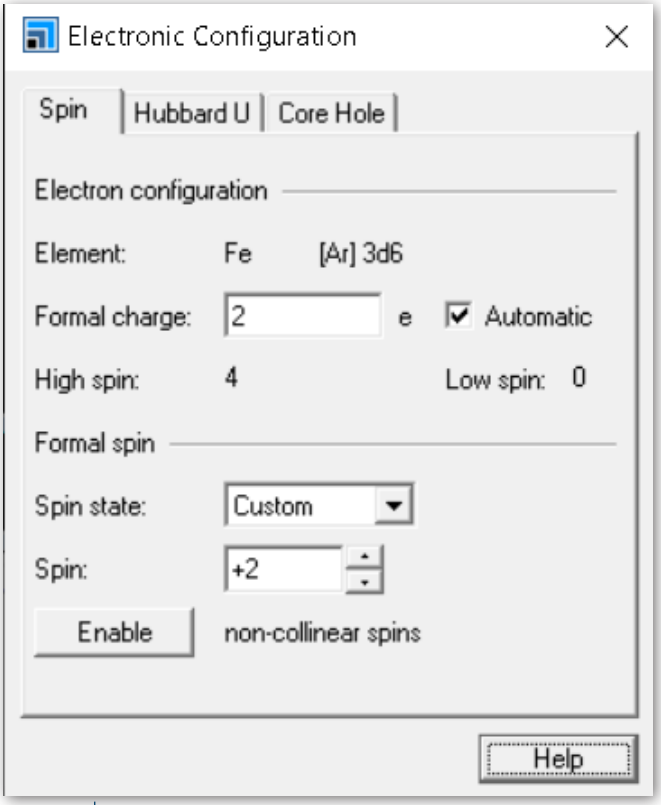

Figure 9: New Collinear spins option is available from the CASTEP Electronic Configuration dialog.

DMol³

New Property! ! The fracture toughness estimate calculated using an empirical model of Niu et al. (2019) for brittle materials is now included in the results of elastic coefficients calculations in DMol³.

ONETEP

New Parameters! We have implemented a family of hybrid functionals.

New Materials! We have extended implicit solvent calculations to include the Poisson-Boltzmann scheme, which allows the inclusion of electrolyte ions as point charges that do not interact with each other but contribute to the screening of solutes.

Updated Solver! We have updated the module to use the academic release version 6.1.1 of the code.

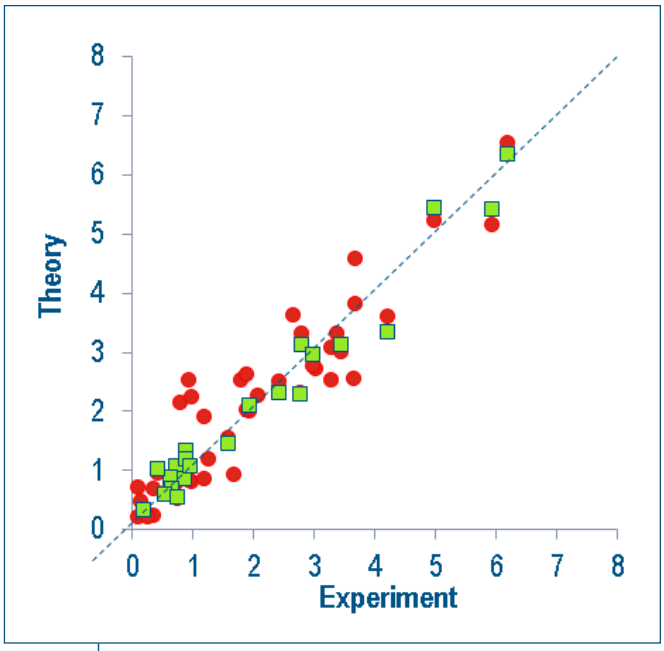

Figure 10: Niu et al. (2019) established a correlation between fracture toughness KIC and elastic properties. The implementation into CASTEP and DMol³ provides access to good quantitative estimate of hardness for brittle ceramic and ionic materials. (Red dots = Using Materials Studio, Green squares = Niu et al. results).

OTHER MODULES

Cantera

Upgraded Solver! We have updated Cantera to version 2.4.0 and Python to version 3.8.1.

ENHANCEMENTS TO PIPELINE PILOT MATERIALS STUDIO COLLECTION

Metal Alloy Protocols

Improved accuracy! We have added vibrational energy contribution to the CALPHAD thermodynamic database calculations.

New Protocol! A new Grain Growth (PhaseField) protocol provides a facility to simulate the growth of alloy grains using the phase-field method.

New Protocol! A new Solidification (PhaseField) protocol provides a facility to simulate the solidification of alloys using the phase-field method.

Polymer Protocols

New Protocol! We have added a protocol to calculate the adhesion energy of a composite system.

New Components! Mesocite Energy, Geometry Optimization, Dynamics, Shear, and Dissipative Particle Dynamics (DPD). New mesoscale structure builder components support structure creation from templates and structure packing into rectangular boxes.

New Protocol! We have expanded the collection by adding a new protocol to create a polymer network using bead models.

Enhanced Performance! Classical simulation using Forcite or Mesocite and including Forcefield fitting protocols now have a parameter "Use GPU" which can accelerate the calculation by enabling the use of a GPU.

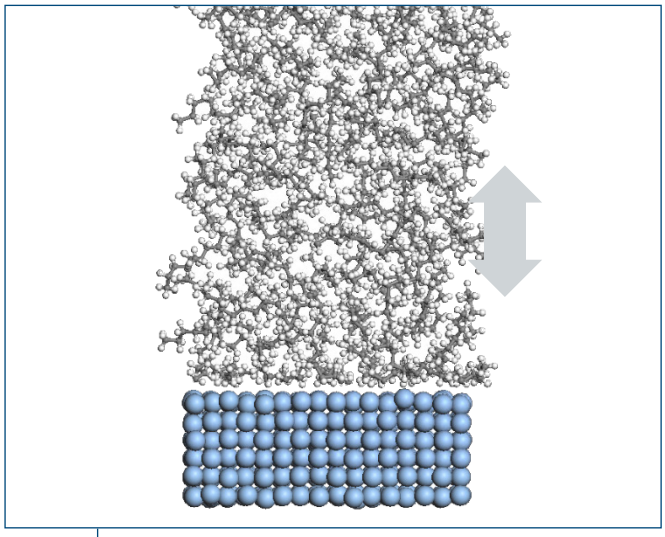

Figure 11: You can screen adhesion energy between layers using a dedicated Pipeline Pilot protocol.

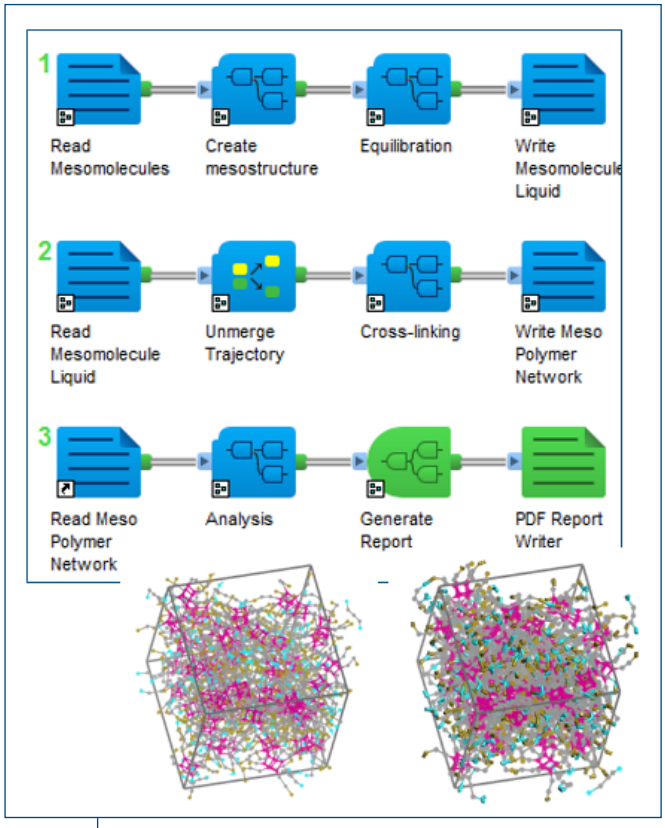

Figure 12: You can build networks of polymers for use in coarse-grained simulations using this new Pipeline Pilot protocol.

Battery Protocols

New Materials! We have added components and example protocols providing access to the external database of experimentally determined crystal structures (Crystallography Open Database) and to the external database of computed crystal data in Materials Project.

Example Protocols

New Protocol! We have added a protocol to calculate Thermal Conductivity to Prototype Examples that implements the Reverse Non-Equilibrium Molecular Dynamics method.

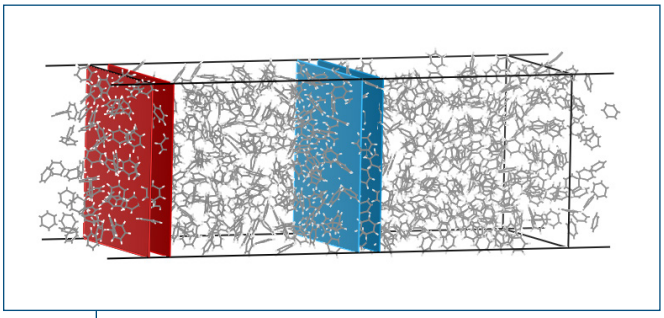

Figure 13: Illustration of a simulation setup for the thermal conductivity protocol now available in Materials Studio Collection 2021.

PLATFORM SUPPORT CHANGES

Platform support added

Server support added for the following configurations:

- Red Hat Enterprise Linux 8.1 and 8.2
- CentOS 8.1 and 8.2

Queuing system support added for:

- Slurm Workload Manager 20.02.x

Single GPU compute support added for:

- NVidia cards that support Compute Capability 6.0 or higher and with CUDA version of 10.1

Platform support discontinued

Server support discontinued for:

- Windows Server 2012 R2

Queuing system support discontinued for:

- Slurm Workload Manager 18

Browser support discontinued for:

- Internet Explorer 11

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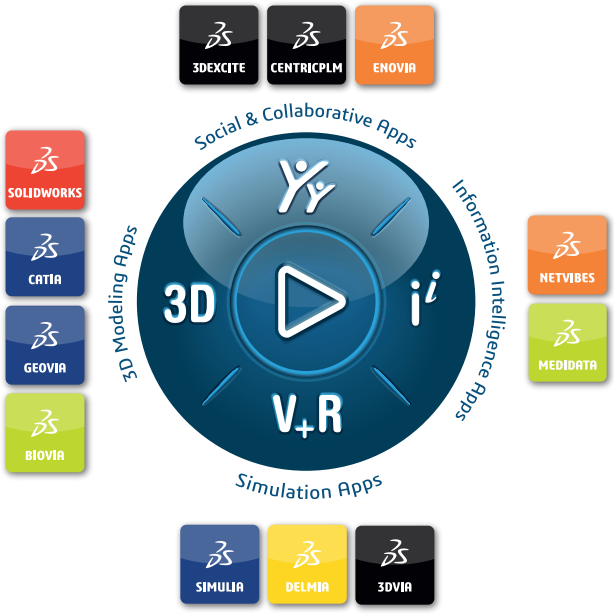

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