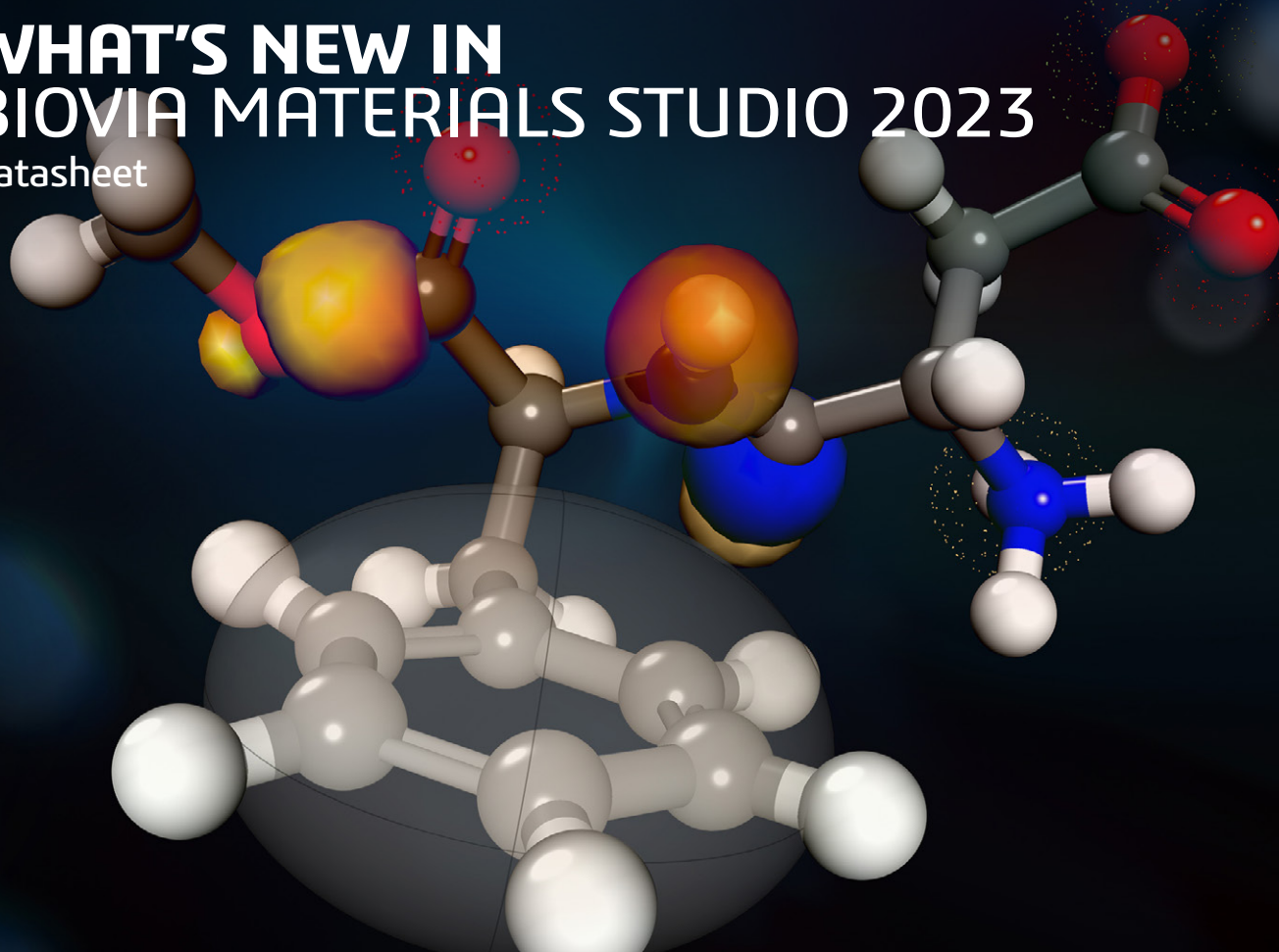**35 BIOVIA**

# WHAT'S NEW IN
# BIOVIA MATERIALS STUDIO 2023
## Datasheet

BIOVIA Materials Studio 2023 is the newest version of BIOVIA's modeling and simulation 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 properties.

The latest release provides scientists with extensive suite of world class solvers and parameter sets operating from quantum to microscales. This release contains enhancements across the full range of solvers, with added convenience for coarse-graining atomistic models and substantial performance increases for classical simulations.

BIOIVA Materials Studio 2023 lets you simulate more material properties, more accurately, and more conveniently than ever before.

**35 DASSAULT SYSTEMES**

## BIOVIA MATERIALS STUDIO 2023 FOR COARSE GRAINED SIMULATIONS

### Automatic Coarse Graining and Bead Typing

Coarse-grained molecular dynamics (CGMD), where groups of atoms are represented by a single bead, are an increasingly popular way to probe the structure and properties of soft matter systems from tens to hundreds of nanometers- scales that are otherwise out of reach to regular atomistic simulation. A successful CGMD simulation requires a well validated set of forcefield parameters to describe the interactions of the beads and to allocate each bead the appropriate forcefield types.

Over the past 20 years, the approach of the Martini forcefield [1-3] has proved popular and applicable to a wide range of materials, culminating in a recent Martini 3 version [4,5] that can claim to provide the most accurate representations to date. The Martini 3 forcefield is available to use as part of the Mesocite module and with Materials Studio 2023 a new set of capabilities that automate the coarse-graining of structures from atomistic models. This greatly simplifies what can be a complicated step to assign bead types provided by Martini 3. This has the double benefit of efficiency in building models and in reducing bead typing errors. These tools are accessible both from new scripting menus and also in the form of Pipeline Pilot protocols in the Materials Studio Collection. The inclusion of protocols make configuring a customized coarse-graining procedure extremely efficient.
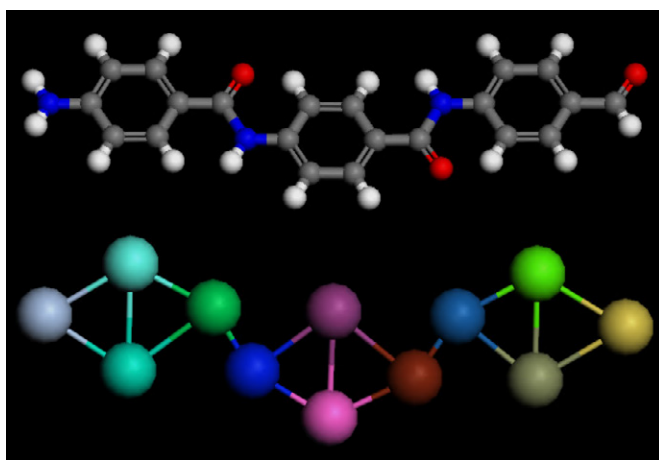


**Figure 1:** Atomistic and bead representations for polymers with hinged structures. The coarse graining tools automatically identify these configurations.

### New Tools!

Martini 3 tools have undergone improvement and now features a new MS Martini 3 Coarse Grainer function. This generates a mesostructure model directly from an atomistic model (see Fig 1) including bead mapping and forcefield typing by using a single template study table. A template file of customized interactions can be specified through the Materials Studio Visualizer such as those shown in Figure 2. These templates allow complex cases, such as hinged structures involving rings to be represented (where quite often the bead centers do not reside on atom centers).

A customized MS Martini 3 forcefield including all the required valence terms is provided along with the mesostructure models, ready for simulation with Mesocite. Mesocite coarse-grained molecular dynamics also benefit from significant acceleration when used with NVIDIA GPUs.
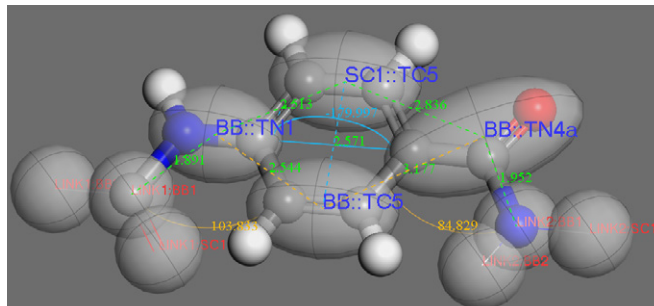


**Figure 2:** Templates are used to provide molecule specific interaction terms to the forcefield file generated by the coarse-graining tools.

### New Tutorial!

A new tutorial demonstrates the use of the Coarse Grain and Generate Custom Martini 3 Forcefield Protocol. This works through the steps required to build mesostructure starting from an all-atom model, creating custom bead mapping templates and generating the coarse-grained structure and the customized MS Martini 3 forcefield.

Material Studio 2023 offers state-of-the-art tools for coarse-grained simulation, speeding up the process of setting up mesoscale materials models.
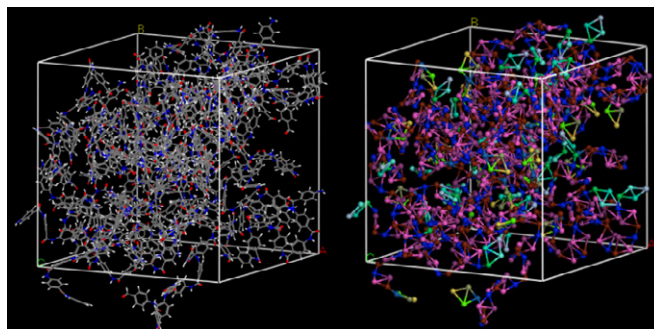


**Figure 3:** Representation of equivalent atomistic and coarse-grained polymer structures.

## Mesocite Dissipative Particle Dynamics

Dissipative Particle Dynamics (DPD) is a popular and proven method to study soft condensed matter self-assembly processes in polymer mixtures, surfactant systems and more. The soft potential approach embodied in DPD provides a very efficient way to reach thermodynamic equilibrium states of the systems. Important subclasses of these materials include polyelectrolytes and charged surfactant systems and with Materials Studio 2023 these are more accurately represented through the inclusion of electrostatic interactions between charge beads within Mesocite DPD.
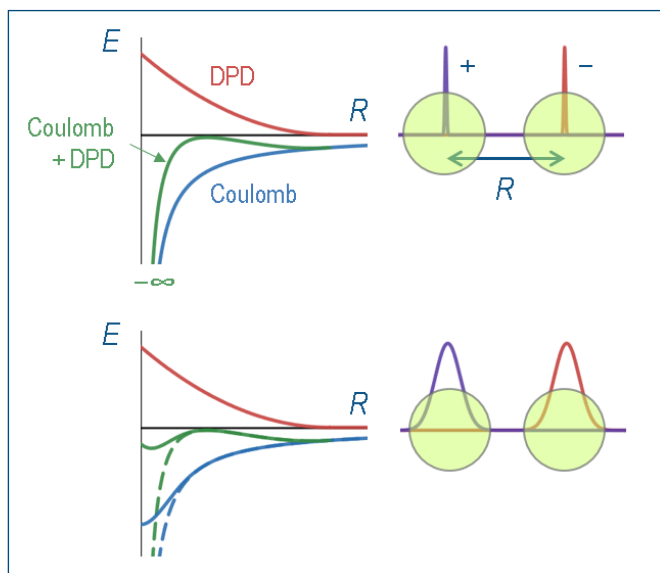


**Figure 4:** Representations of interaction energies between unlike charges in DPD both without (top) and with (bottom) Gaussian smearing of charges.
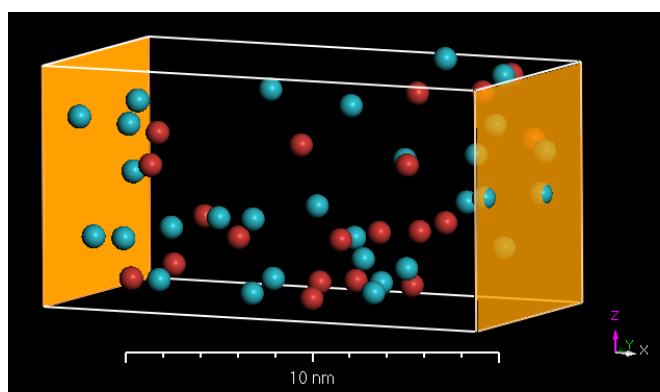


**Figure 5:** Models demonstrating the distribution of charged beads in a salt solution near a charged plate.

Mesocite DPD now supports electrostatics by allowing the smearing of bead charges using a Gaussian distribution of charge. This avoids the collapse of unlike charges to a singularity as DPD beads (represented by soft finite potentials) pass through each other.

With Materials Studio 2023 you can also benefit from faster dynamics by running Mesocite DPD on NVIDIA GPUs and the addition of two new analysis features:

- Calculation of the structure factor from a density field.
- Pressure analysis that provides anisotropic components.

In Materials Studio 2023, the Mesocite DPD module provides new functionality and at a greater speed for simulating more systems.

## BIOVIA MATERIALS STUDIO 2023 FOR METAL ALLOY DESIGN

BIOVIA Materials Studio PhaseField, based on OpenPhase_Core solver was introduced in Materials Studio 2021 for simulating hard material microstructures. With PhaseField module, you can conveniently define the component phases, grain set up, thermodynamic and kinetic input, and temperature and pressure conditions, through an easy-to-use interface in the Pipeline Pilot Connector. This allows phase transitions in multicomponent metal alloys to be studied in detail.

Being able to accurately predict phase transitions is a key to improving the quality of metal components created using the additive manufacturing process. The size and shape of metal grain microstructures are highly sensitive to the rate at which the liquid metal solidifies during the printing process. Different proportions of crystal phases can emerge during solidification which ultimately impact the material properties. New features for studying these transformations are provided in Materials Studio 2023 and include:

### New Protocol!

A new protocol to calculate continuous cooling transformation (CCT) diagrams is provided that can be used to predict the critical cooling rate for the alloy. This protocol can make use of co-installed ThermoCalc or OpenCalphad package to provide the CALPHAD thermodynamic input.

### New Feature!

The Time-Temperature-Transformation (TTT) Diagram protocol now fits and returns Johnson-Mehl-Avrami (JMA) coefficients for each simulation temperature. The JMA model describes how solids transform from one phase to another at a constant temperature.
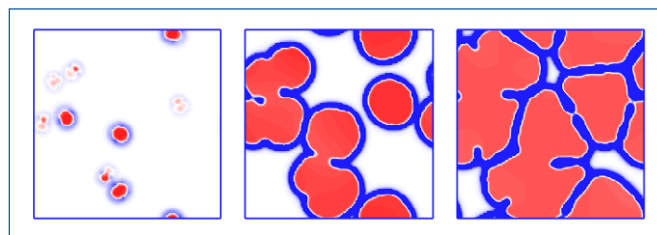


**Figure 5:** Images showing stages of solidification in a metal alloy PhaseField simulation.

## BIOVIA MATERIALS STUDIO 2023 FOR CHEMICAL REACTIONS

Materials Studio already provides a broad suite of tools and features to understand chemical reactions through; application of quantum mechanical solvers, DMol³ CASTEP, DFTB+ and VAMP; application of chemical transition state searching using FlexTS module; and reaction kinetics predictions (Cantera and Kinetix modules). Materials Studio 2023 provides further capabilities for the scientist using Materials Studio to understand chemical reactions by way of access to TURBOMOLE, and the beyond DFT methods it provides.

### New Protocols!

A set of protocols that provide TURBOMOLE workflows through the Pipeline Pilot Protocols dialog are now available which provides DFT, xTB and Wavefunction methods

- Single-point energy calculation for all methods
- Geometry optimizations (using xTB, DFT or MP2)
- Transition state optimizations (using xTB or DFT)
- IR spectra / Vibrational frequencies (using DFT)
- Polarizabilities (using DFT)
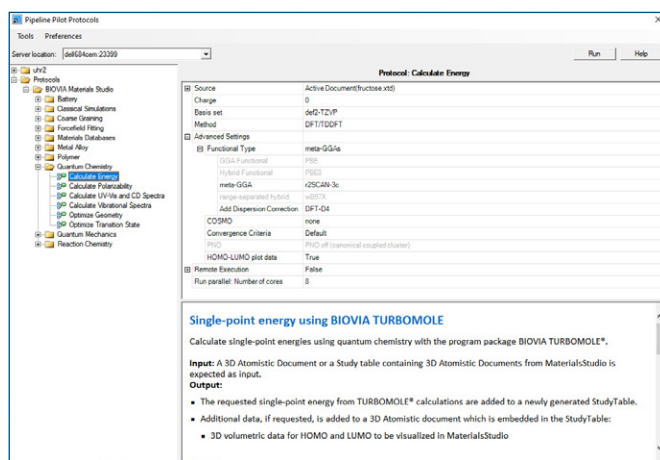- Optical spectra (using DFT)

**Figure 6:** TURBOMOLE protocols can now be run through Pipeline Pilot Materials Studio Collection protocols.

### New Utilities!

Protocol enhancements now make it simpler to construct customized workflows for automating reactive simulation studies

- A new "Edit Sets" component allowing you to create and manage sets in Pipeline Pilot
- Scripting now recognizes SMILES and chemical names for molecules and fragments
- A script to analyze the content of a simulation cell or the development of different reagents over the course of a trajectory is available from a new scripting menu
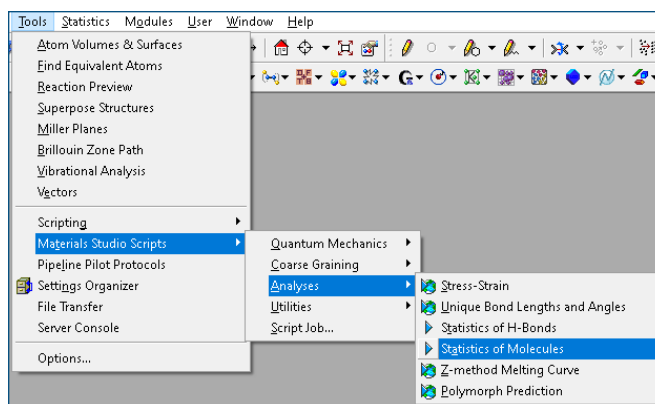
**Figure 7:** New tools are available from a Materials Studio Scripts menu, including an analysis of simulation box contents.

## BIOVIA MATERIALS STUDIO 2023 FOR XPS SPECTROSCOPY

XPS (X-ray photoelectron spectroscopy) measures an excitation (binding) energy of a core electron in a molecule or periodic structure. A new tool is available in Pipeline Pilot Materials Studio Collection 2023 to conveniently provide the spectra. The protocol also provides for convenient assignment of an offset through calculated or experimental data.
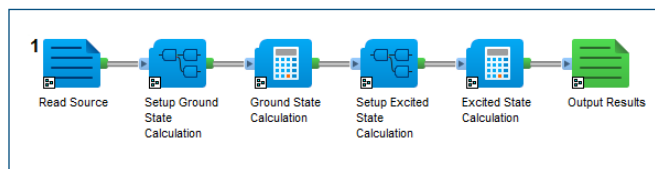
**Figure 8:** The XPS protocol automates the production of XPS spectra from CASTEP calculations.

## MATERIALS STUDIO MODULE ENHANCEMENTS

### Classical Simulations
### Enhanced Performance! More Parameters!

- **Solver Features**
  - Mesocite DPD now supports electrostatics by allowing the smearing of bead charges using a Gaussian distribution.
- **Solver Performance**
  - Forcite GPU calculations now support the Embedded Atom Model.
  - A review of the Forcite dynamics GPU algorithms has resulted in updates providing significant performance enhancements.
  - You can now run Mesocite Dissipative Particle Dynamics (DPD) calculations on NVIDIA GPUs.

- **Analysis**
  - Mesocite and Forcite analysis now support calculation of the structure factor from a density field.
  - Mesocite and Forcite analysis now support pressure analysis with anisotropic components.
- **Parameters**
  - The COMPASSIII water model now provides a much improved prediction of diffusion coefficients and surface tension. Predicted values are now close to experimental accepted values.
  - MS GULP is now equivalent to academic v6.1.
  - A periodic version of the novel universal forcefield GFN-FF is now implemented in GULP. This is a fully automated polarizable forcefield with nearly quantum-mechanical accuracy, as described in [6].

### Quantum Mechanics –More Parameters! More Properties!

- **CASTEP**
  - A new protocol for calculating core-level XPS spectra and absolute electron binding energies.
  - Linear response calculations of vibrational properties for spin-polarized (magnetic) systems.
  - CASTEP DFT+U no longer requires a spin-polarized setting for systems that actually are not magnetic, making such calculations at least a factor of two faster.
  - Force calculations in the presence of implicit solvent are now available in CASTEP. This allows you to perform geometry optimization, molecular dynamics, and other tasks taking into account the effect of solvents.
- **DFTB+**
  - Upgrade to version 22.1
  - New libraries of DFTB+ parameters for Ti oxides and for Ce oxides
  - COSMO implicit solvation model is implemented.
- **ONETEP**
  - Upgrade to version 6.1.12
  - Hybrid exchange-correlation functional implementation for 3D periodic systems

### MATERIALS STUDIO PRODUCTIVITY ENHANCEMENTS

#### Enhancements to Pipeline Pilot Materials Studio Collection

The Pipeline Pilot Protocols dialog provides access to enhancements available in the Materials Studio Collection for Pipeline Pilot, including:

- A new set of Quantum Chemistry protocols that provide TURBOMOLE workflows.
- A Quantum Mechanics protocol that allows you to calculate XPS spectra.

- A utility protocol for selecting atoms and editing sets.
- Enhancements to the Coarse Graining protocols.
- Improvements to the PhaseField protocols.

### Enhancements to MaterialsScript

- Scripting now recognizes SMILES and chemical names for molecules and fragments. A script to analyze the content of a simulation cell or the development of different reagents over the course of a trajectory is also available.
- You can now access wide range of prepared MaterialsScript tools from Tools > Materials Studio Scripts in the menu bar. These scripts were previously provided as examples to manually add to the User menu.

### Materials Studio Infrastructure

- On Linux, you can now configure and use SSH for communication between the Materials Studio client and server.

### TUTORIALS

The following new tutorials have been added or updated

- **Polymer Coarse Graining with Martini 3 Tools and Mesocite:** Demonstrates how to generate templates for bead mapping, use templates with the Martini 3 Coarse Grainer, and customize the MS Martini 3 forcefield for a given polymer structure.
- **Polymer Coarse Graining with Martini 3 Protocols:** Demonstrates how to generate templates for bead mapping, use templates with the Coarse Grain and Generate Custom Martini 3 Forcefield protocol, and customize the MS Martini 3 forcefield for a given polymer structure.
- **Calculating the Minimum Energy Path of a molecular switch.**
- **Calculating the properties of diamond.**

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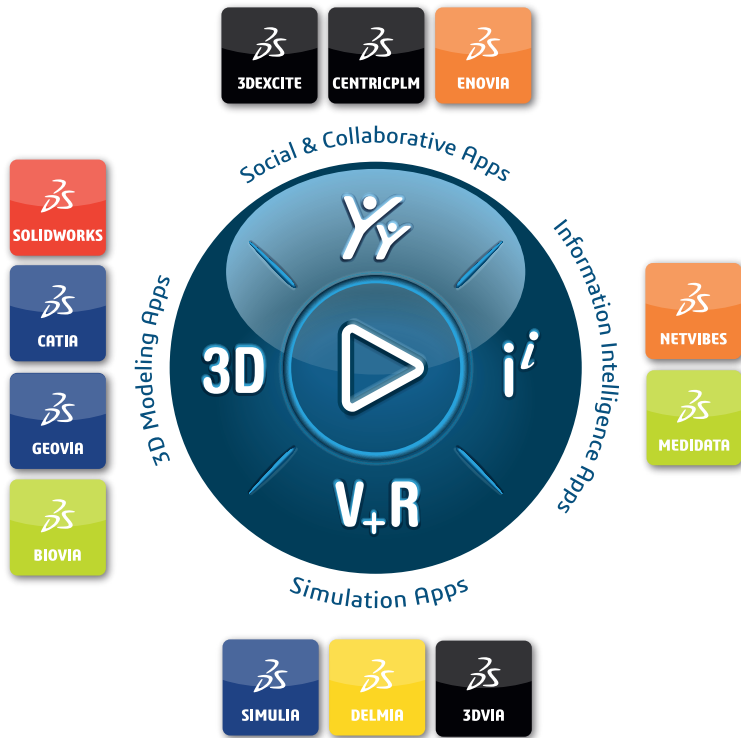
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