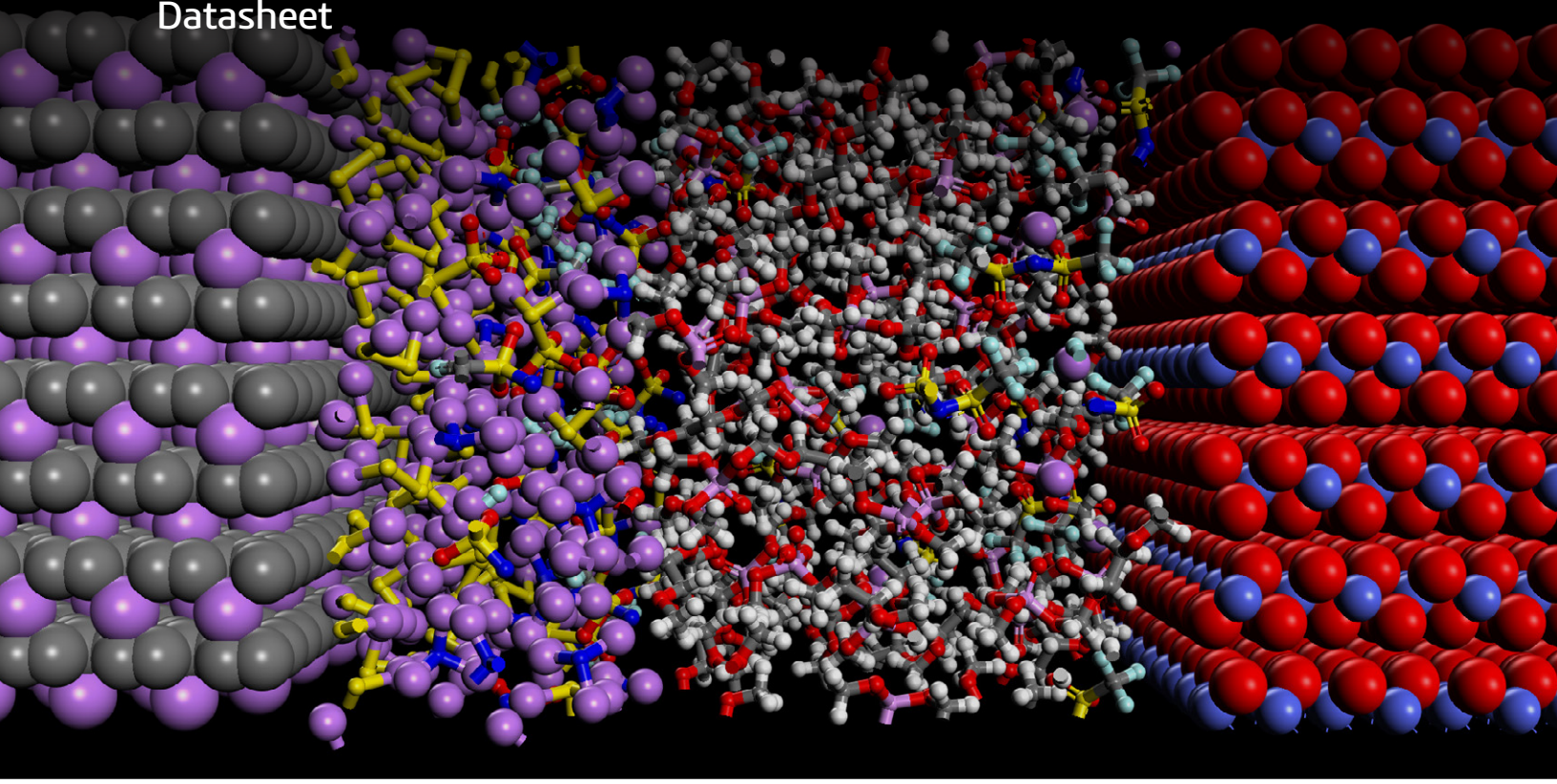
# WHAT'S NEW IN
# BIOVIA MATERIALS STUDIO 2020

Datasheet



BIOVIA Materials Studio 2020 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 in order to make more informed decisions about materials research and development.

More often than not materials performance is influenced by phenomena at multiple scales. Scientists using Materials Studio 2020 have an extensive suite of world class solvers and parameter sets operating from atoms to microscale for simulating more materials and more properties than ever before. Furthermore, the predicted properties can now be used in multi-physics modeling and in systems modeling software such as SIMULIA Abaqus and CATIA Dymola to predict macroscopic behaviors. In this way multiscale simulations can be used to solve some of the toughest problems in materials design and product optimization.

## BETTER MATERIALS - BETTER BATTERIES

Safe, fast charging batteries with high energy density and long life are urgently needed for a host of applications - not least for the electrification of all modes of transportation as an alternative to fossil fuel energy sources. Battery design relies on a complex interplay between thermal, mechanical and chemical processes from the smallest scales of the material (electronic structure) through to the geometry of the battery cell and pack design. Improvements to the component materials used in batteries and capacitors are fundamental to providing the advances in performance needed.

Materials Studio provides new functionality to enable the simulation of key materials parameters for both liquid electrolytes and electrode components.

1. **New Protocol!** A new "Mass and Charge Transport" protocol in the Materials Studio Collection has been added to allow for calculation of mass and charge transport properties of complex electrolyte solutions. It is specifically configured for liquid battery electrolyte formulations and returns the characteristics of lithium ion transport needed to run systems level battery cell models, such as those provided by CATIA Dymola [1]. Electrolyte formulations may now be optimised using ultimate battery cell performance as one of the criteria.
2. **New Protocol!** A second protocol for calculation of the open circuit voltage from the insertion of ions into electrode structures has been added to the Materials Studio Collection. This is configured to use the insertion of lithium into the stable models of candidate anode materials (E.g. C, Si, Ge) or into complex cathode materials, but any ion can be used. In the case of the multicomponent cathode materials, they can be accurately represented using structures generated by cluster expansion method (also available in the Materials Studio Collection). The "Open-Cell Voltage" protocol returns the half-cell potential difference characteristic, of the material using the ion supplied. The protocol uses CASTEP by default, but runs on any server where the total energy is supplied.

## METAL ALLOYS – FROM DENSITY FUNCTIONAL THEORY TO CALPHAD DATABASES

The structure of metal alloy materials is characterized by complex grain structures which arise from the different stable atomic crystal phases they contain. These phases reflect the lowest energy configurations that appear as a function of composition, temperature and pressure and can be predicted using cluster expansions and related methods based on density functional derived energies. These methods tackle the combinatorial problem of accurately representing complex mixtures of metals. BIOVIA Materials Studio Collection already contains a convenient and extensive set of tools to generating these structures, based on ATAT tools [1]. A new capability for the 2020 release extends this further to use the set of stable crystal structures and simulations of the liquid phase to generate a CALPHAD database in TDB format. Metastable phases can also be included to improve the coverage of the phases that should be included.

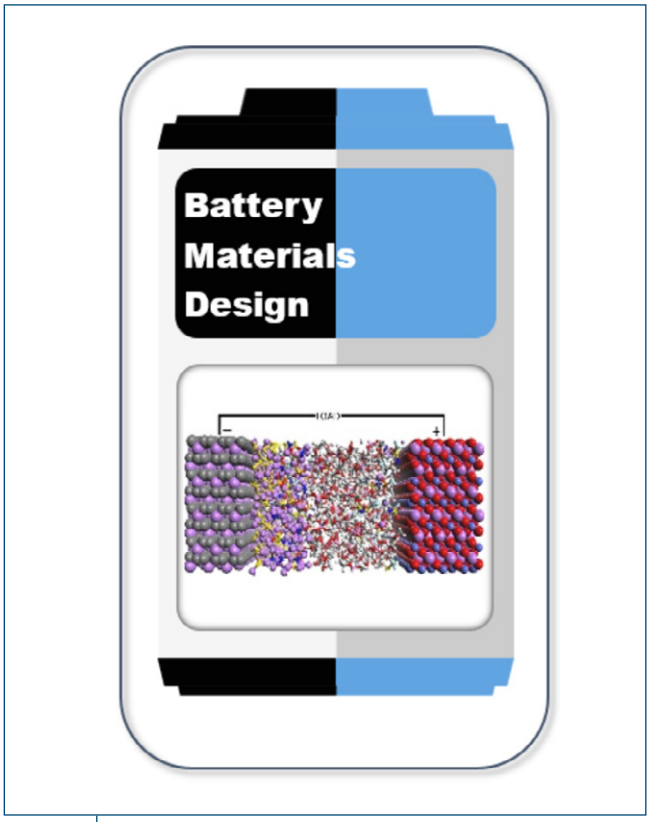



**Figure 1:** Cartoon image of atomistic battery models showing electrodes, electrolyte and SEI layers.

CALPHAD (Computer Coupling of Phase Diagrams and Thermochemistry) databases provide a convenient way to capture the Gibbs free energy in multi-component phase space and enable phase diagrams to be plotted using programs such as Pandat [2], ThermoCalc [3] and FactSage [4].

Using the powerful toolkit for metal alloys in BIOVIA Materials Studio Collection it is now possible to explore the phases expected to occur during solidification of in-silico designed alloy materials.

TBD formatted files may also be used to supply Phase Field simulation codes with the input required to accurately represent the development of grains and dendrites themselves. As such the CALPHAD database is an important bridging technology between atomistic and mesoscales for this class of material.

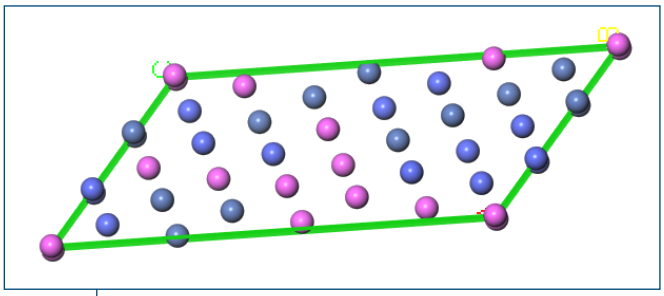


**Figure 2:** Example of a special quasi-random structure (SQS)– typically part of the CALPHAD database creation process.

$$G^{\theta}(y,T) = \left(E^{\theta}_{DFT}(y) - \sum_i x_i E^{\alpha_i}_{DFT}\right) + \sum_i x_i E^{\alpha_i}_{SGTE}(T) - TS_{id}(y,T)$$

**Figure 3:** Expression of Gibbs Free energy as a function of the model phase, $\vartheta$ - fitted independently against DFT total energies for SQS models used to populate the CALPHAD database.

## MORE PARAMETERS – BETTER SCIENCE!

### Classical Simulations

Predictions using classical forcefield based simulations are only as reliable as the parameters describing the interactions between constituent atoms or beads. Where parameters are not explicitly fitted or in the worst case scenario are missing entirely, the outcomes are seriously compromised. In BIOVIA Materials Studio Collection 2020 protocols are now available for carrying out custom fitting of new parameters.

**New Protocol!** For valance parameters (bond stretch, angle bend and torsions), automatic fitting to energies and forces determined by DMol³ is encoded into a single Pipeline Pilot protocol.

**New Protocol!** A second is configured to fit van der Waals parameters to condensed phase material properties.

Detailed tutorials are included to walk through worked examples for adding new parameters. The parameterizations can be launched direct from Materials Studio via the Pipeline Pilot Connector.

**New Parameters!** BIOVIA Materials Studio COMPASS[5] has long been regarded as a world leading force-field for supporting classical simulation of multiple classes of materials. Materials Studio 2020 marks the release of the next generation of these parameters, COMPASS III[6], making use of automated fitting procedures and with improved ionic liquid support. COMPASS III is the result of fitting thousands of common structures found in Maybridge[7], PoLyInfo[8] and ILThermo[9] databases to produce high quality parameters for a wide range of materials.

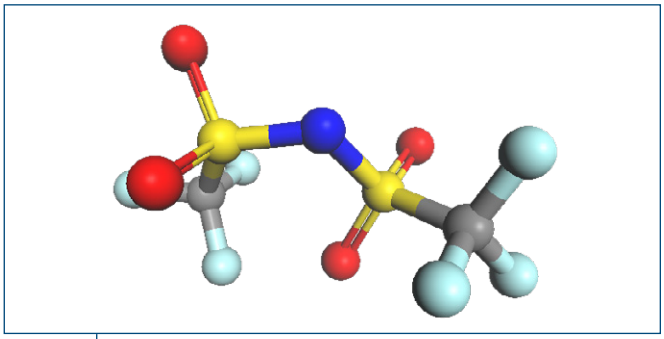


**Figure 4:** Bis[(trifluoromethyl)sulfonyl]imide – the lithium salt of this ionic liquid, a popular Li-ion battery electrolyte, has been refitted for COMPASS III.

### Quantum Mechanics - DFT Functionals

**New CASTEP Functional!** The RSCAN Meta-GGA functional[10] has been added to BIOVIA Materials Studio CASTEP. This is a regularized version of the recent general purpose SCAN functional[11], that eliminates some instabilities found in the original implementation. RSCAN is transferable and accurate for a broad range of solid state and molecular systems. It can be used for phonon calculations using finite displacements method and for NMR properties (except for J-Coupling).

**More DMol3 Functionals!** In DMol³ additional hybrid functionals have been exposed based on implementing the standard libXC library. The available options now include PBE0, TPSSh, SCAN0, M06 and M06-2X. They are available for execution of DMol³ within QSAR, QMERA and the Materials Studio Collection.

### DFTB+ Parameterization

**New Scripts!** Scripts for automating DFTB+ parameterization procedures are available in the Examples/Scripting folder of your Materials Studio installation. These dramatically simplify the process of creating both the electronic and repulsive parts of Slater-Koster files for a set of element pairs. A tutorial "Creating parameters for DFTB+" is available to describe the steps needed in detail.

### COSMO-RS COSMOBase

**New Feature!** An option has been added for running DMol³ COSMO with settings that are consistent with DMol³-PBE COSMOBase. It is now possible create COSMO files using Materials Studio and transfer them for use in COSMOtherm[12]. BIOVIA COSMOtherm implements COSMO-RS theory for accurate calculation of solubilities, activity coefficients, phase diagrams, vapor pressures, heats of vaporization and phase equilibria for both pure fluid and liquid mixtures.

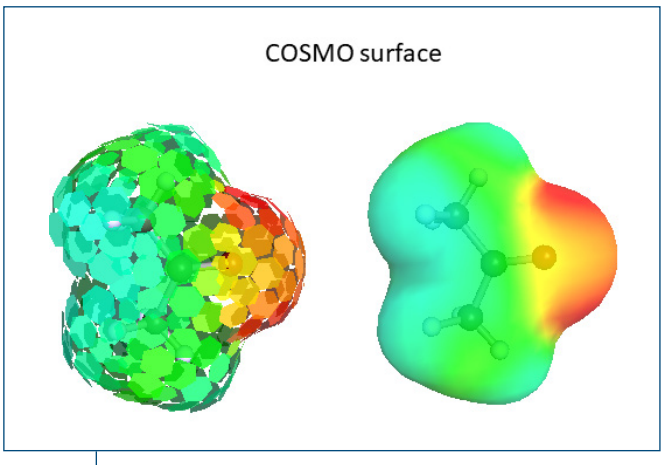



**Figure 5:** COSMO surfaces representation.

## LARGE METALLIC SYSTEMS

**New Feature!** BIOVIA Materials Studio ONETEP has been extended to provide linear scaling modeling of large metallic systems. The Annealing and QUenching Algorithm for Fermi Operator Expansion (AQUA-FOE) method [13] has been successfully applied to modeling large nanocluster models on thousands of cores, for development of new catalyst materials.[14]

## PERFORMANCE & USABILITY

**New Feature!** A multiple time step method has been added to Forcite, which is now the default for calculations using Ewald and PPPM electrostatics. The reciprocal space part of the electrostatic calculations is done on every fourth time step, which has little to no impact on the accuracy of calculated energies. but affords a significant improvement in performance for multiprocessor calculations.

**New Feature!** When running calculations through the Pipeline Pilot Connector in Materials Studio, you can now reuse the settings from a previous protocol to populate the input fields.

**New Protocol!** Components have been added to the Materials Studio Collection to add the ability to run LAMMPS [15] molecular dynamics directly from BIOVIA Materials Studio. An example protocol using this component has also been provided.

## PROPERTIES & ANALYSIS

### COOP/COHP analysis

**New Feature!** Crystal Orbital Overlap and Crystal Orbital Hamiltonian Population analysis has been added to DMol$^3$. This makes it possible to analyse bonding in molecular crystals. COOP/COHP can be used as the indicator of strength of bonding by orbital energy and can be used to can resolve DOS into bonding/anti-bonding density of states.

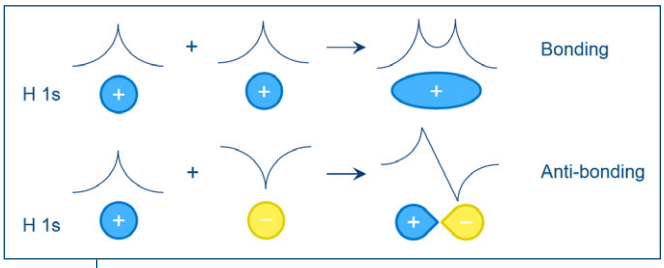



Figure 6: Bonding/anti-bonding nature of molecular orbitals is of interest to chemists. COOP/COHP analysis makes the same insights possible for crystal systems.

### Forcite & Mesocite

- **New Feature!** Concentration Profile analysis now outputs the profile as mass density in g/cm$^3$ in addition to standard concentration profiles.
- **New Feature!** Trajectory analysis now also computes diffusion coefficients directly by automatic fitting to the means square displacement data when there is sufficient statistics to do so.
- **New Feature!** Forcite dynamics now supports oscillatory electric fields via the MaterialsScript API.

**New Script!** A Materials Studio script is now available that implements the so called Z-method [16], a way to estimate the melting temperature of crystal models, in particular metals, at different pressures. The script can be found in the Examples/Scripting folder of the Materials Studio installation.

## OTHER MATERIALS STUDIO 2020 HIGHLIGHTS

### CASTEP

- The CASTEP user interface has been significantly modified to reflect the current state of the server code and to aid usability.
- The EPR task is now used when requesting G-tensor in NMR properties, so that the hyperfine tensor is produced in a G-tensor calculation. Documentation for the calculation of hyperfine tensor has been made more explicit.
- The Vibrational Analysis tool can now be accessed from IR spectrum selection on the CASTEP Analysis dialog.
- The library of on the fly generated potentials for high-throughput studies (library QC5) has been made available in Materials Studio scripting.
- Visualization of electrostatic potentials, including workfunction calculations, is now available in CASTEP for hybrid exchange-correlation potentials.

### GULP

- A simulated annealing task has been added to GULP to provide flexible control over temperature in molecular dynamics simulations.
- GULP server code has been updated to the academic version 5.2 where the main changes in functionality are:
  - Multiple temperature ramps allowed in MD for simulated annealing.
  - Dipolar polarizability (in the limit of non-interacting dipoles) now has second derivatives.
  - Domain decomposition allowed for general unit cells instead of just orthogonal and monoclinic.
  - Finite strain derivatives added.
  - Spin added as a species attribute in order to support Ising models along with J2 and J3 coupling.
  - Surface energy calculations added for MEAM.
  - Improved smoothing of lone pair and over-coordination energies added in ReaxFF.
  - Option to add a shear force included.
  - Output of eigenproperties of the elastic constant added.
  - Baskes potential now has tapering in two-body component.
  - MEAM-2nn-QEq library extended to include parameters for Li-Co-O and Ti-O/Si-O systems.

## ONETEP

- Local DOS analysis in conjunction with the optimization of conduction states is now supported by the ONETEP user interface.
- A solvation model with periodic boundary conditions is now implemented in ONETEP, to support modeling of bulk and surface systems in a solvent.
- Electron localization function analysis is now available in ONETEP, as a way of visualizing the nature of bonding in large systems.
- Time dependent DFT calculations of electronic excitations in ONETEP are now possible with the PAW potentials, in addition to the previously available option of using norm-conserving pseudopotentials.

## QMERA

- Calculation of Raman spectra using DMol$^3$ has been added to QMERA.

## QSAR

- The VAMP Electrostatics model in QSAR can now be used to calculate dipole moments in the zero differential overlap approximation (ZDO). This is in addition to the previously available natural atomic orbitals or point charges (NAO/PC) approximation.

## Tutorials

The following new tutorials have been added:

**NEW! Fitting valence forcefield parameters using Pipeline Pilot:** Demonstrates how to run the Fit Valence Parameters protocol in the Materials Studio Collection for Pipeline Pilot from Materials Studio.

**NEW! Fitting non-bond forcefield terms using using Pipeline Pilot:** Demonstrates how to run the Fit VDW Parameters protocol in the Materials Studio Collection for Pipeline Pilot from Materials Studio.

**UPDATED! DFTB+: Creating parameters for DFTB+:** A new section on identifying good electronic settings has been added.

A number of tutorials have also been to use 2020 features such as COMPASS III parameters.

- **DMol3**: Kinetics of a Diels-Alder reaction
- **Forcite**: Calculating the diffusivity of a gas in a polymer
- **Pipeline Pilot Connector**: Cross-linking polymers usin Pipeline Pilot
- **Pipeline Pilot Connector**: Calculating the stress-strain diagram using Pipeline Pilot
- **Reflex**: Structure solution of 4-nitrophenylhexylurethane using a close-contact penalty

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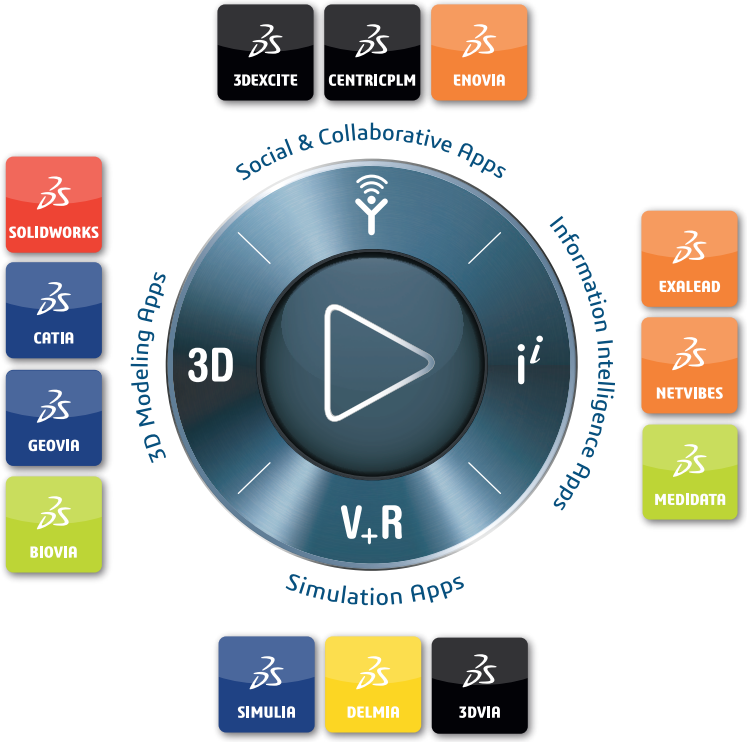


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