WHAT'S NEW IN
BIOVIA MATERIALS STUDIO 2022
Datasheet

3DEXPERIENCE®

BIOVIA Materials Studio 2022 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 2022 have access to an extensive suite of world class solvers and parameter sets operating from atoms to microscale. This release extends and enhances the two recently introduced modules: FlexTS, for transition state searching and PhaseField for hard material microstructure prediction. In addition you can benefit from further performance improvements in classical simulations on CPU and GPU and make use of the new Martini 3 coarse-grained forcefield.

With BIOIVA Materials Studio 2022 you can simulate more material properties, more accurately, and more efficiently than ever before.

## BIOVIA MATERIALS STUDIO FlexTS WORKFLOWS FOR REACTION KINETICS

Based on the code developed at the University of Cambridge [1-5] BIOVIA Materials Studio FlexTS was introduced in Materials Studio 2021 to provide robust chemical 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, subsequently calculate the transition states, and locate 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+.

In Materials Studio 2022 the following enhancements have been made:

- **Improved Performance!** DMol[3] Minimum Energy Path calculations now run in-process, significantly improving computational performance by minimizing start up and completion processes.

- **Enhanced Usability** In DMol[3] Minimum Energy Path and DFTB+ Minimum Energy Path calculations you can now:
  - Conveniently inspect intermediate NEB trajectories and convergence results
  - Start calculations from an existing trajectory.

With knowledge of transition states obtained from FlexTS, you can use the reaction kinetics task in Dmol[3] to provide rate coefficients that are in turn inputs for BIOVIA Materials Studio Cantera and BIOVIA Materials Studio KINETIX modules. With BIOVIA Materials Studio 2022 chemists and chemical engineers have a powerful, robust and flexible suite of methods to bridge from quantum mechanics to chemical reaction kinetics.

- Efficient, numerically stable and easy to use transition state searching
- Multiple options for reaction pathways, TS refinements and reactions with low barriers
- Study reactions using multiple tools (DMol[3], DFTB+, FlexTS, Reaction Preview, Reaction Kinetics, Kinetix and Cantera) within the single Materials Studio environment.
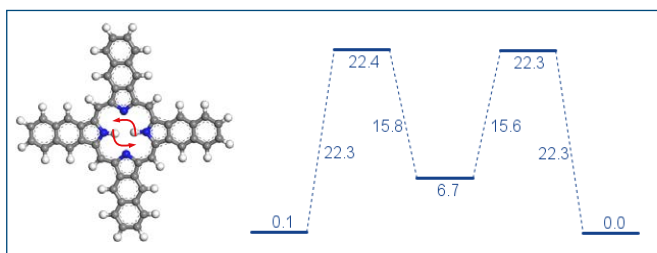
Figure 1: Images of an example multistep reaction treated by FlexTS and the corresponding reaction pathway energy levels as computed by use of DFTB+. You can graph the reaction pathway by processing the FlexTS output in a dedicated Pipeline Pilot Protocol in the Materials Studio Collection.
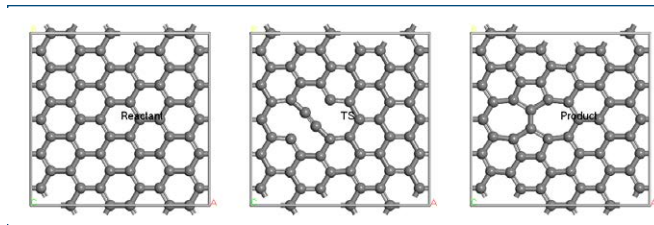
Figure 2: Images depicting the reaction, transition state and product of a Stone-Wales defect formation barrier in graphene.
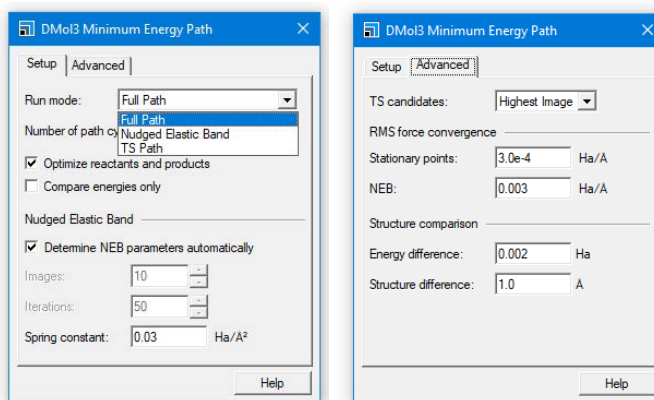

Figure 3: Dialogs showing new tasks available in DMol[3] for running FlexTS tasks.

BIOVIA MATERIALS STUDIO PHASEFIELD WORKFLOWS FOR METAL ALLOY DESIGN

BIOVIA Materials Studio PhaseField, based on OpenPhase_Core solver [6-8] was introduced in Materials Studio 2021 for simulating hard material microstructures. 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.

One important application of these simulations is for optimization of metal additive manufacturing. BIOVIA Materials Studio PhaseField can be used to understand dependence of microstructure on the print conditions during powder bed fusion additive manufacturing. Individual layers of metal alloy powder are melted and solidified leading to transformations between crystal phases which are sensitive to both the cooling rate and local temperature. This dependence is captured by time-temperature-transformation (TTT) diagrams. In Materials Studio 2022 you can create TTT diagrams with a dedicated Pipeline Pilot Materials Studio Collection protocol. The TTT output provides key parameters of macroscopic simulations of the printing process that can be executed using SIMULIA Abaqus models.

With BIOVIA Materials Studio 2022 materials scientists and metallurgists can bridge to the macroscopic world of metal casting and additive manufacturing from the first principles prediction of metal alloy mixtures at atomistic scales.
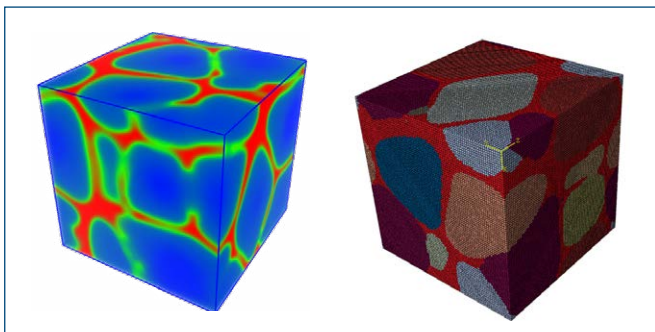
Figure 4: Two example microstructure outputs from BIOVIA Materials Studio PhaseField simulation showing the boundaries between grains. The first is a field density from BIOVIA Materials Studio and the second shows a voxel representation inside SIMULIA Abaqus software.
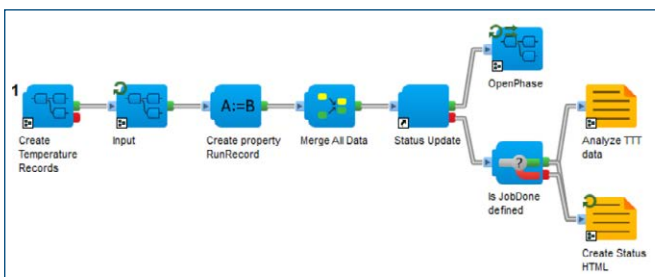
Figure 5: Materials Studio PhaseField simulations can be automated by assembling components in Pipeline Pilot. Here a TTT (time-temperature-transformation) diagram is constructed from a series of individual phase-field calculations

MATERIALS STUDIO MODULE ENHANCEMENTS

Classical Simulations
Enhanced Performance! More Materials!

In Materials Studio 2021 support for NVIDIA GPU processors brought substantial performance benefits to both the highly functional classical molecular dynamics methods in Forcite and coarse-grained simulations in Mesocite. Materials Studio 2022 provides you with further performance improvements on both GPU and CPU and these benefits are also now available in Pipeline Pilot Materials Studio Collection protocols that use Forcite and Mesocite.

Coarse-grained simulations are increasingly popular for extending the length and time scales accessible by classical molecular dynamics. With Materials Studio 2022 you can run coarse-grained simulations for a wide variety of materials with increased accuracy using the recently developed Martini 3 forcefield [9]. Preparation of the systems is made more convenient with new user scripts that apply Martini 3 bead typing and you can learn about this in a new tutorial in the Materials Studio Help.

- **New Parameters!** The new MS Martini 3 provides access to the Martini 3 forcefield
- **Improved Usability!** Preparation tools for bead-based structures and specialized custom MS Martini 3 forcefields associated with them.
- **New Tutorial!** A new tutorial demonstrates how to customize the MS Martini 3 forcefield and use it to generate a bead topology file for molecules.
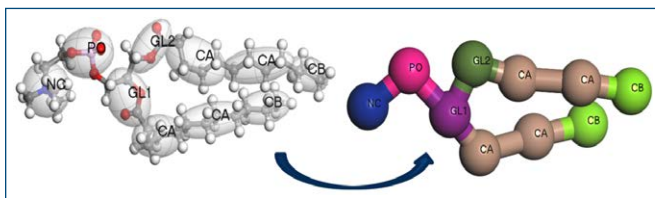

Figure 6: You can assign Martini 3 forcefield types as part of coarse-graining steps using new user scripts in Materials Studio 2022.

Classical Simulations
Reactive Forcefields

Regular classical molecular dynamics does not change the bonding topology of the molecules, but there are systems where incorporating chemical changes is required to accurately represent how the material composition can evolve over time. One approach to achieve this is to identify possible reaction sites from reactant molecules and periodically update the bonding networks according to specific stochastic rules. In Materials Studio 2022 you can make use of a collection of perl scripts (deployed in a perl module called ReactionFinder) to build reactive molecular dynamics capabilities. With ReactionFinder functions reaction sites can be identified and bonding networks updated as part of custom scripts. You can explore these new features by following two new tutorials.

- **New Tutorial! Executing Virtual Atomistic Reactions with ReactionFinder:** Helps you to learn how to use ReactionFinder to execute virtual reactions.
- **New Tutorial! Using ReactionFinder to Simulate the Formation of the Solid Electrolyte Interphase:** Demonstrates how to use ReactionFinder as part of a larger Monte Carlo-Molecular Dynamics hybrid algorithm. Simulating the complex and long-timescale reactive behavior of an anode-electrolyte interface at which an SEI forms.
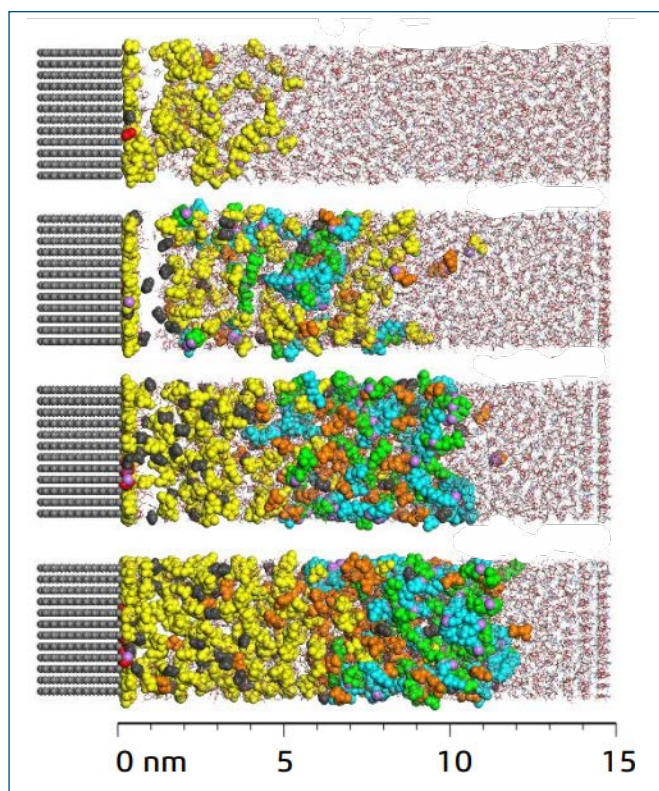
Figure 7: You can assign apply new ReactionFinder methods to build reactive molecular dynamics simulations using hybrid Monte Carlo/Molecular Dynamics. In this example a Lithium ion battery solid electrolyte interphase structure is constructed at the surface of a graphite anode.

Quantum Mechanical Simulations

Updates to solvers based on quantum mechanical methods include the following enhancements,

- **New Parameters!** You can now run calculations using the MBD* dispersion correction scheme if you provide custom parameters in CASTEP.

- **New Properties!** You can now calculate piezoelectric coefficients using the Berry phase approach in CASTEP.

- **Enhanced Usability!** DMol3 Scripting now returns the .cosmo file in the scripting hash for calculations using the COSMO solvation model.

- **Increased Accuracy!** The version of DFTB+ has been upgraded to version 20.2.1 providing more accurate forces.

- **New Settings!** Spin relaxation is now available in spin-polarized DFTB+ calculations, to allow you to search for the true magnetic ground state of molecules and solids.

- **New Parameters!** Grimme D4 dispersion corrections are now available in DFTB+
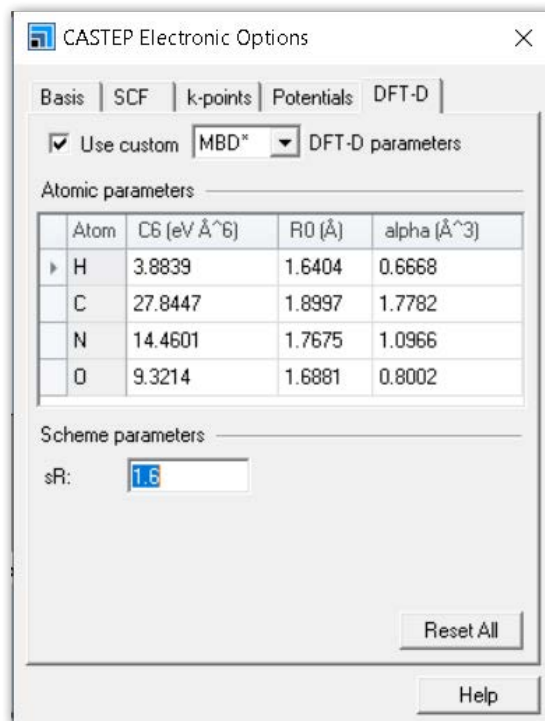
Figure 8: CASTEP GUI now allows user to enter custom parameters and run any DFT-D with the RSCAN functional

PLATFORM SUPPORT CHANGES

Platform support added

- Server support has been added for Red Hat Enterprise Linux 8.3 and 8.4
- Queuing system support has been added for:
  - Altair Portable Batch System (PBS) Pro 2020.x and 2021.1.x
  - Slurm Workload Manager 20.11.x and 21.08.x
- Browser support has been added for: Mozilla Firefox ESR 78 or later

Platform support discontinued

- Server support has been discontinued for CentOS 8.x
- Queuing system support has been discontinued for:
  - Slurm Workload Manager 19.05
  - Adaptive Computing TORQUE 6.1.2
- Browser support has been discontinued for: Mozilla Firefox ESR 68

REFERENCES

1. Munro, L. J.; Wales, D. J. "Defect Migration in Crystalline Silicon," *Phys Rev* B, **59**, 3969-3980 (1999).

2. Carr, J. M.; Trygubenko, S. A.; Wales, D. J. "Finding Pathways between Distant Local Minima," *J. Chem. Phys.*, **122**, 234903-234910 (2005).

3. Wales, D. J.; Carr, J. M "Quasi-Continuous Interpolation Scheme for Pathways between Distant Configurations," *J. Chem. Theory Comput.*, 8(12), 5020–5034 (2012).

4. Kumeda, Y; Munro, L. J.; Wales, D. J. "Transition States and Rearrangement Mechanisms from Hybrid Eigenvector-Following and Density Functional Theory. Application to C10H10 and Defect Migration in Crystalline Silicon," *Chem. Phys.* Lett., **341**, 185-194 (2001).

5. Trygubenko, S. A.; Wales, D. J. "A Doubly Nudged Elastic Band Method for Finding Transition States," *J. Chem. Phys.*, **120**, 2082-2094 (2004).

6. Steinbach, Ingo "Phase-field models in materials science," Modelling Simul. Mater. Sci. Eng. 17 (2009) 073001.

7. Steinbach, Ingo "Why Solidification? Why Phase-Field?," JOM 65 (2013) 1096–1102.

8. OpenPhase_Core. http://openphase-solutions.com

9. P.C.T. Souza, et al., Martini 3: a general purpose force field for coarse-grained molecular dynamics, Nat. Methods, 18, 382-388 (2021).

Our **3D**EXPERIENCE® Platform powers our brand applications, serving 11 industries, and provides a rich portfolio of industry solution experiences.

Dassault Systèmes, the **3D**EXPERIENCE Company, is a catalyst for human progress. We provide business and people with collaborative virtual environments to imagine sustainable innovations. By creating 'virtual experience twins' of the real world with our **3D**EXPERIENCE platform and applications, our customers push the boundaries of innovation, learning and production.

Dassault Systèmes' 20,000 employees are bringing value to more than 270,000 customers of all sizes, in all industries, in more than 140 countries. For more information, visit **www.3ds.com**.

DASSAULT SYSTEMES | The **3D**EXPERIENCE® Company

DS-9989-0122