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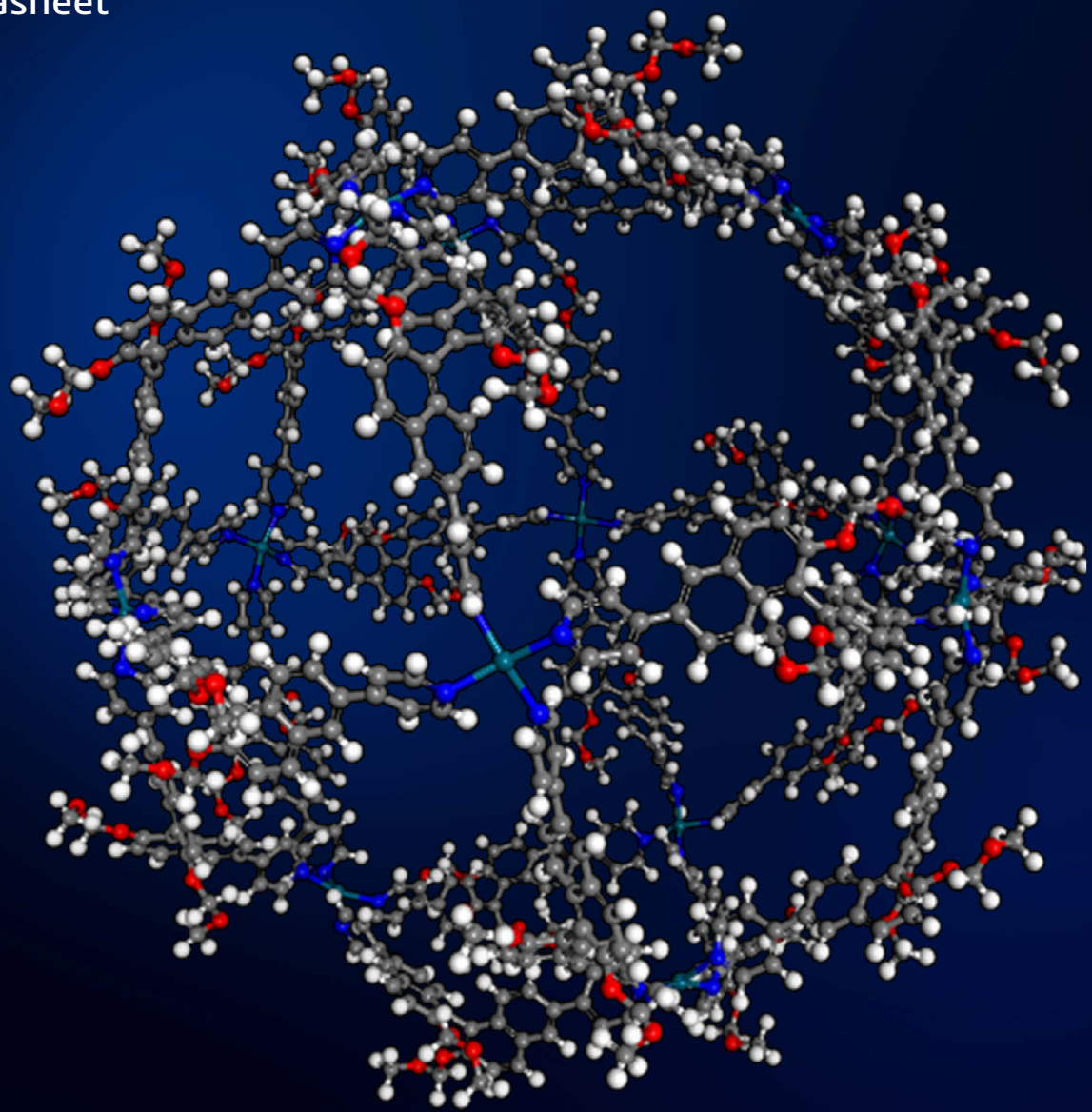
WHAT'S NEW IN MATERIALS STUDIO 2026

Datasheet



DASSAULT SYSTEMES

BIOVIA Materials Studio is BIOVIA's predictive science tool for chemistry and materials science research. The latest release of Materials Studio empowers researchers to get an even deeper understanding of the relationships between the material's molecular or crystal structure, its properties and possible chemical reactions. Scientists using **BIOVIA Materials Studio 2026** have access to an extensive suite of world class solvers and parameter sets operating from quantum to microscales.

This release marks a milestone in the over twenty-five years history of Materials Studio as Python is now included as one of the native scripting languages alongside Perl. This opens up the possibility to create complex workflows in Python and to integrate Python libraries adding a vast range of additional functionality for manipulating molecules and machine learning.

This release also contains a range of enhancements; the range and usability of the machine learned force field MACE has been extended and there are also tools to customize and fine-tune the MACE potentials with new data to obtain high quality results for your system.

Additionally, the implementation of the FlexTS algorithm for transition state search in Forcite together with the enhancements of MACE now enables you to investigate chemical reactions for much large systems with an accuracy comparable to quantum mechanics. A new script changes the calculation of the viscosity from an estimate to being predictive.

Materials Studio 2026 is faster than ever. The calculation of IR-spectra prediction and the use of non-local exchange functionals in CASTEP is enhanced. An increasing number of the modules like Forcite and CASTEP run on GPUs and the new standard solver for DFTB+ is GPU accelerated.

With these advances, you can simulate a larger variety of material properties, more accurately, and quicker than ever before.

SCRIPTING FOR AUTOMOTION OF COMPLEX WORKFLOWS IN MATERIALS STUDIO

Python Scripting in BIOVIA Materials Studio 2026

MaterialsScript is a vital part of Materials Studio enabling you to automate any operation ranging from low level tasks, like manipulating molecules to running complex computational workflows. MaterialsScript has been based on Perl, but the 2026 release turns Materials Studio bilingual as it introduces Python as an additional scripting language.

Scripting in Materials Studio

The computational modules in Materials Studio provide high precision calculations of physical properties. However, some properties are more elaborate to calculate, may need combinations of properties and also require to calculate averages over ensembles or time. These types of calculations and also the generation of the models can be programmed into a workflow via scripting.

Python

Python is a versatile language for scripting and there are many libraries available for download at repositories. It has established itself as the standard language for machine learning and it is the most used programming language over all according the TIOBE Programming Community index [1]. The Python interpreter component and a Jupyter Notebook component has been available in Pipeline Pilot, but Python is now available also in **Materials Studio 2026** as a native Materials scripting language.

Features and Capabilities

The MaterialsScript Python interface shown in Fig. 1 enables you to write and debug Python code in the Materials Scripting Editor and to execute the Python code on any server via the Gateway. The MaterialsScript implementation of Python supports all the built-in functionality in Materials Studio Visualizer for manipulating molecules and solids to create atomistic models, to run jobs with the computational modules and perform analysis on the results. It covers all functions described in the Python Built-in Functions documentation [2]. It also supports all the standard Python library modules described in the Python Standard Library documentation [3], accessible through the import statement. Downloading additional Python libraries gives the possibility to extend the functionalities in Materials Studio to generate complex structures, perform analysis and even run machine learning in a Materials Script.

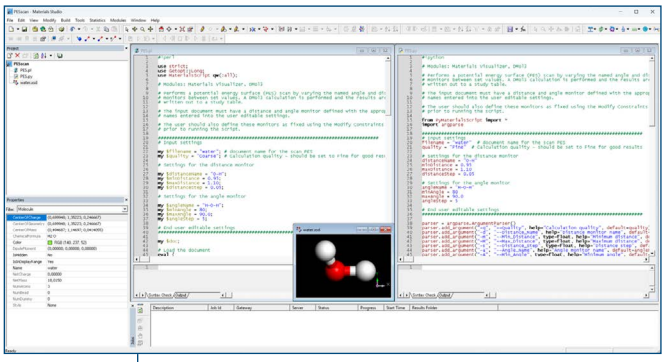


Figure 1: Materials Studio 2026 supports two languages, Perl and Python, such that Python code can be written and debugged in the MaterialsScripting Editor and executed via the Gateway.

BIOVIA MATERIALS STUDIO 2026 FOR ADVANCED SIMULATIONS

Materials Studio 2026 Continues to Improve the Machine Learned Forcefields

Machine Learned Interatomic Potentials (MLIPs) are force fields that are trained on quantum mechanical data. MLIPs don't have predetermined bonds, but the interactions are based on the potential energy surface derived from Density Functional Theory (DFT) calculations. This means that MLIPs can, in contrast to classical force fields, treat bond breaking and chemical reactions in a similar way as quantum chemical calculations, but with a much reduced calculation time.

Two New Versions of MACE are Available in Materials Studio 2026

Two versions of the MACE (message passing or multi-atomic cluster expansion) MLIPs [4] were introduced in the 2025 release, MACE-OFF23 and MACE-MP-0. **Materials Studio 2026** introduces a new version called MACE-MATPES-r2SCAN-0 [5]. This MLIP is aiming to be a general force field for solid state systems. It was first trained on the Open Materials (OMat24) database provided by Meta and further fine-tuned on the MatPES data set, which is a recalculation of a subset of the Materials Project database using the r2SCAN exchange-correlation functional. The MACE-MP-0 force field has been replaced by the MACE-MP-0b3, which is extended to be a full foundation model [6]. A foundation model can be used a starting point for further fine-tuning by training with user data. The new Pipeline Pilot protocol "MACE Fine Tuning" enables you to start from one of the MACE force fields and create your own tailormade force field for your system by fine-tuning.

Dispersion Correction for Van-der-Waals Bonded Systems

Standard DFT calculations do not by default include the long-range van-der-Waals interactions, but can be corrected via a dispersion correction. The MLIPs may include the dispersion correction at the training stage or as an extra term during the molecular dynamics simulations. Both approaches have been used in the training procedure of MACE. MACE-OFF23 aimed at molecular simulations was trained with dispersion corrected DFT data. The MACE-MP-0b3 and MACE-MATPES-r2SCAN-0 force fields derived for solid materials were trained on data without information about vdW-interaction, so they would need a dispersion correction during the MD-simulations. The molecular dynamics module Forcite can now use the D3 dispersion correction [7] together with MACE potentials in order to correctly describe solid systems held together by vdW-interactions. This is very important to obtain correct density and crystal structure for Active Pharmaceutical Ingredients (API) that crystallize into molecular crystals and layered materials that are used as anode and cathode materials in batteries. Fig. 2 shows how the D3 dispersion correction improve the results for the prediction of the volume contraction in the battery cathode material NMC811 during charging.

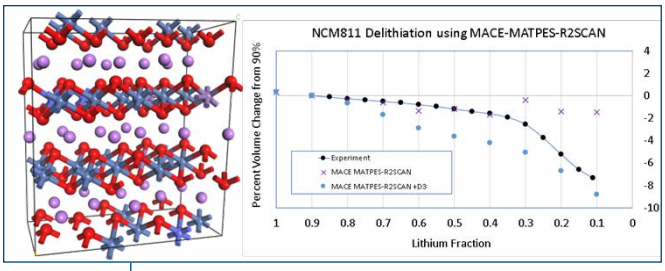


Figure 2: The volume contraction of the layered battery cathode material NMC811 ($LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$) during charging. The values are calculated with the MACE-MATPES-r2SCAN-0 force field with and without the D3 dispersion.

UNDERSTANDING THE CHEMISTRY IN COMPLEX SYSTEMS

BIOVIA Materials Studio 2026 Takes a Quantum Leap in Chemistry

Materials Studio 2026 is opening up the possibility to investigate chemical reactions in much larger systems. The activation barrier is a crucial to properly understand the reaction kinetics in any chemical process. Locating the exact transition state requires both a very accurate method to calculate the potential energy surface and an intelligent way to map out the reaction path. This combination of requirements has limited the range of systems that can be investigated to small to medium sized molecular systems that can be treated by quantum mechanical methods in CASTEP or DMol^3.

Study Chemical Reactions with Forcite

The Forcite module is now able to investigate chemical reactions in a similar way as the quantum modules, but at lower computational cost. Significantly larger systems can be addressed or multiple reaction paths may be mapped out very quickly. The potential energy surface at transition states can be calculated by MLIPs like MACE and by using the FlexTS-based Minimum Energy Path task (Fig. 3a) the precise location and energy of the transition state can be determined. This enables you to investigate reactions in complex systems like polymerization reactions, catalytic reactions in homogeneous or heterogeneous environments and electrochemical reactions in a battery cell. Fig. 3b) shows that the diffusion path and the energy barrier for lithium diffusion in silicon calculated with MACE-MATPES-r2SCAN-0 force field agrees well with both fullscale DFT calculations and experimental data.

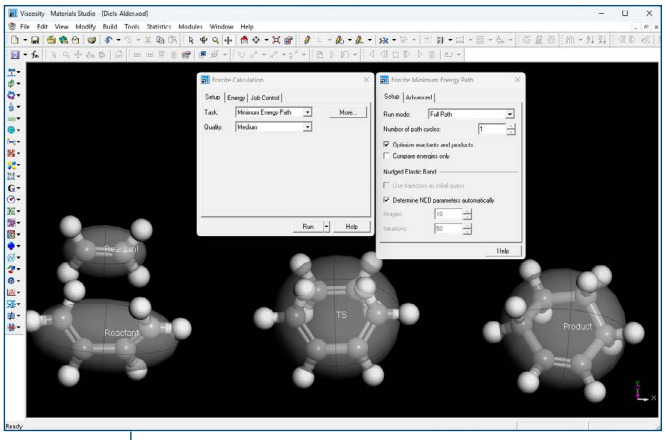


Figure 3a: The setup of a Minimum Energy Path Task for molecular reactions in Forcite.

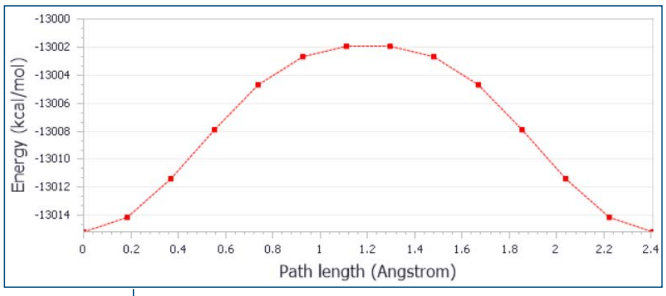


Figure 3b: The diffusion path for lithium in a silicon anode material calculated with the Minimum Energy Path method in Forcite using the MACE-MATPES-r2SCAN-0 force field. The calculated diffusion energy barrier agrees very well both with full DFT calculation with CASTEP and experimental measurements.

MATERIALS STUDIO 2026 FOR LIQUID SYSTEMS

Calculate the Viscosity of Your Formulation

Viscosity is a fundamental property alongside density for the performance of fluid formulations. The smearing ability of lubricants is intimately connected to the viscosity of the mixture of oils. Getting the right thickness is as well vital for any formulation in the Consumer Package Goods (CPG) industry, ranging from ketchup to shampoo to creams. However, it takes time to measure the viscosity with a viscosimeter and it becomes an increasingly tedious task to optimize the viscosity for a complex formulation. Fortunately, the viscosity depends on the interaction between the molecules in the fluid, so it can be calculated by molecular dynamics.

Materials Studio 2026 introduces a new workflow to calculate the viscosity as can been seen in Fig. 4a) and 4b). The standard approach to calculate viscosity via the stress autocorrelation requires very long molecular dynamics simulations to obtain reasonable results for the predicted viscosity. The new tool for viscosity prediction is instead using an ensemble average over multiple starting configurations. The averaged simulation data is finally fitted to a double exponential function. This approach increase the accuracy of the predicted viscosity and it is faster. In particular as it can be coarse grained parallelized.

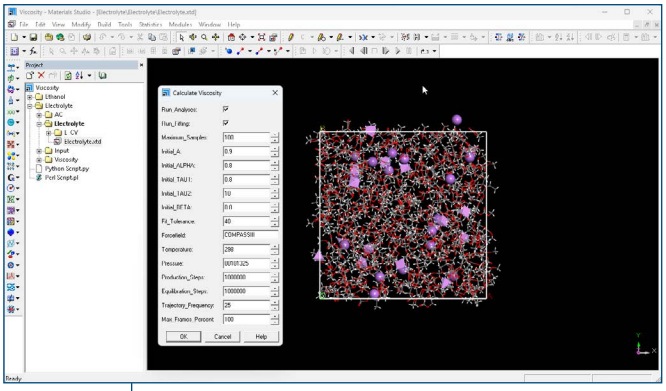


Figure 4a: The setup dialog for the Viscosity workflow script to calculate the viscosity for a fluid formulation.

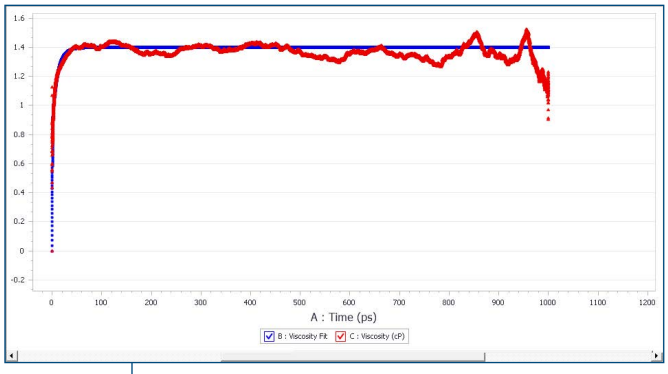


Figure 4b: The convergence of viscosity value in a typical fluid simulation.

MATERIALS STUDIO 2026 FOR SOLID SYSTEMS

Improved Speed for CASTEP and DMOL

The quantum mechanical simulation codes for solid systems, CASTEP and DMol³ are very accurate, but compute intensive. **Materials Studio 2026** introduces a number of new features that enhance the computational speed and accuracy of these modules.

Automatic Improvement of the Job Settings

The iterative process to find the ground state in DFT calculations is sometimes difficult to converge. CASTEP or DMol³ jobs that fail to converge SCF iterations or geometry optimization can be configured to be resubmitted with adjusted parameters such that the calculations have an improved chance of converging.

Predict IR-spectra Solid Systems

Infrared spectroscopy (IR) is a well-established technique to identify chemical groups via their vibration modes. However, connecting the peaks in the IR-spectra to particular structural features requires measurements of reference samples, where these structural features are present in an unambiguous way. It is therefore convenient to be able to calculate theoretical IR-spectra as reference. These have the additional advantage to allow to directly observe the vibration movement of the atoms for a particular vibration frequency in the calculated IR-spectra to characterize the vibration mode. The IR-spectra simulations have been resource consuming in CASTEP, but **Materials Studio 2026** enables to use ultrasoft pseudo potentials to calculate the vibration modes and the IR-intensities. This significantly decreases the computational cost of the IR-spectra prediction with CASTEP. Fig. 5a) demonstrates that the IR-spectra calculated with the new implementation using Ultrasoft pseudopotentials agrees very well with the results from the linear response calculation.

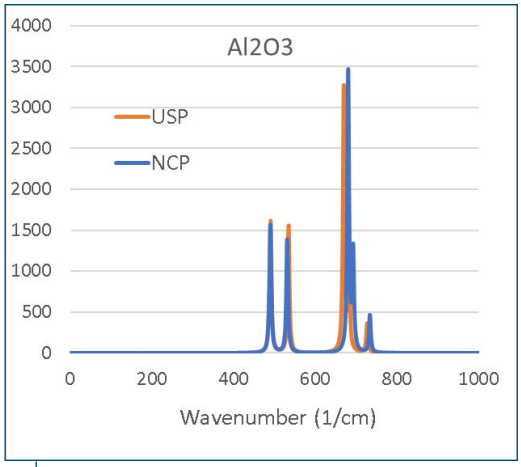


Figure 5a: The Infrared absorption spectra of Al2O3 calculated with CASTEP using the finite displacement method with Ultrasoft Pseudopotentials (USP) compared to the Linear Response formalism and Normconserving pseudo potentials (NCP).

Faster Application of High-Resolution Calculations

How the quantum mechanical exchange and correlation interaction between the electrons in the material is treated determines the quality of the calculations. CASTEP is able to calculate the very accurate nonlocal treatment of the exchange-correlation functionals, but they have been highly resource consuming. The Adaptive compressed exchange, ACE, is a new method that allows CASTEP calculations that use nonlocal or hybrid exchange-correlation functionals to run significantly faster.

Calculate the Actual Hubbard-U Value for Your System

Solid materials like transition metal oxides often have a very strong electron correlation effects that require a Hubbard interaction treatment. The U-parameter in the Hubbard method for the correlation effects is frequently set to a fixed value or it is determined by adjustment until calculated properties fit a target value physical property like the band gap. The U-parameters can also be calculated by a linear response method [8]. Fig. 5b) presents the interface to the new Pipeline Pilot protocol "Calculate Hubbard U Values." This protocol is an implementation to refine U values for DFT+U calculations with CASTEP.

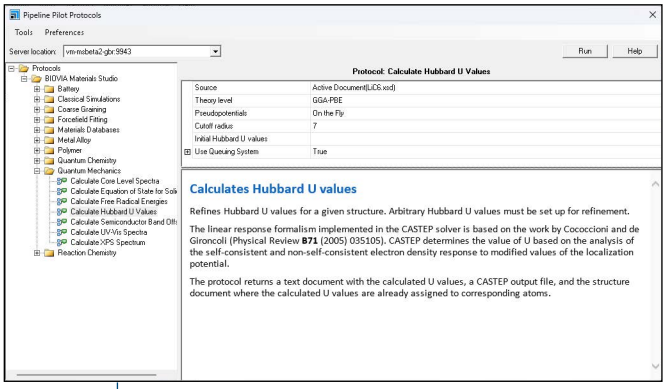


Figure 5b: The Pipeline Pilot Connector interface to setup a calculation of the Hubbard-U parameter with CASTEP using the new protocol "Calculate Hubbard-U values."

MATERIALS STUDIO HIGHLIGHTS BY MODULE

CASTEP

Full coverage of vdW-corrections for all elements in the periodic table: The D3 [7] and D4 [9] CASTEP dispersion correction schemes now include parameters for all elements up to Z=103.

Faster IR-spectra predictions: You can now calculate infrared spectra using ultrasoft pseudopotentials in CASTEP.

Improved convergence: The Materials Studio Gateway can help to automatically restart CASTEP calculations with improved settings if the previous job fails to converge.

Faster calculations with non-local XC-functionals: Accelerate CASTEP calculations that use non-local exchange correlation functionals through use of the Adaptively Compressed Exchange (ACE) method.

COMPASS

New Parameters: COMPASS III now supports tetracoordinate boron compounds (dialkylamino-substituted boranes).

DFTB+

New Slater-Koster Library for crystals: DFTB+ now includes the PTBP (Periodic Table Baseline Parameter) set for solid state modeling [10].

GPU accelerated Eigenvalue solver: The default eigenvalue solver for the DFTB+ module is now ELPA and supports GPU acceleration. The ELPA solver is only supported on Linux servers. In scripting, the eigenvalue solver automatically reverts to Divide and Conquer on Windows servers.

New Tight-binding Hamiltonian: DFTB+ now allows you to use the xTB Hamiltonian through the GFN1-xTB, GFN2-xTB, and IPEA1-xTB parameter sets [11]. Fig. 6 shows that the GFN1-xTB performs well for heat of reactions compared to DFT values.

DMOL³

Better convergence: A new setting to improve calculation settings when DMol³ jobs fail to converge SCF iterations or geometry optimization calculations, such that the calculations converge.

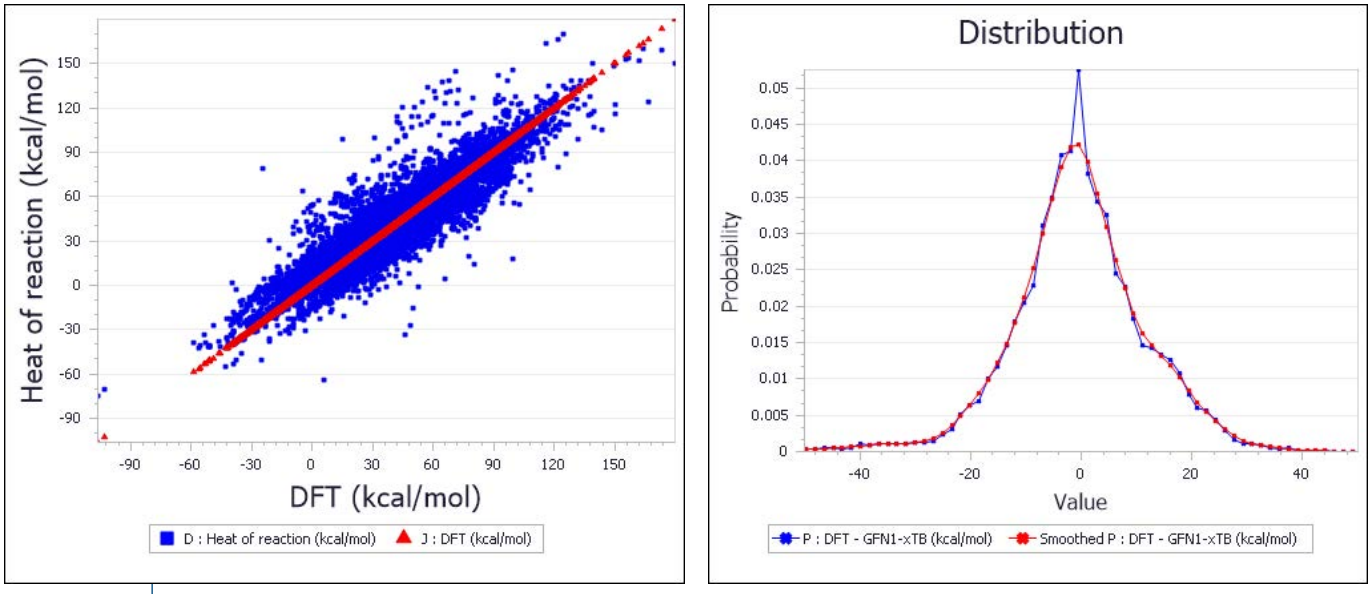


Figure 6: Validation of the heat of reaction for a large set of for molecular reactions calculated with the GFN1-xTB Hamiltonian against DFT data.

FORCITE

Increased Performance for molecular systems: The Forcite GPU implementation of Group based sums has been optimized.

Chemistry for large systems: The Forcite Minimum Energy Path task allows you to compute energy barriers and reaction pathways using the FlexTS module. This calculation is a highly automated and stable transition state search module that requires very little user input. MACE machine-learned forcefields underpin this functionality.

Better Van-der-Waals Interactions: Forcite now implements the D3 model of the dispersion interaction, for use with MACE forcefields.

GULP

Upgraded Solver: The GULP solver now uses academic version 6.4. This version brings new features such as:

- Calculation of anisotropic Grueneisen parameters
- Direct calculation of thermal expansion coefficients
- Addition of triple bond and C2 special terms to ReaxFF
- Support for the ACKS2 algorithm for QEq with analytical first derivatives
- The range of charge equilibration schemes now includes SCQEq, EQEq, and others
- Input files can now control whether to treat H differently in QEq
- Change the coulomb interaction form for QEq to a range of different forms
- Calculation of energy as part of the convergence check during iterative charge solutions.

MATERIALS STUDIO INSTALLER

Support for .7z files: The Materials Studio installer is now provided as a .7z file.

ONETEP

Upgraded Solver: The ONETEP solver code now uses the academic version 7.3.95, in particular this provides improved performance of the fast density mode and a reduced memory footprint. Fig. 7 demonstrates the speed-up with the new Fast solver compared to the standard solver.

Improved calculation speed: You can now optimize ONETEP calculations for speed rather memory.

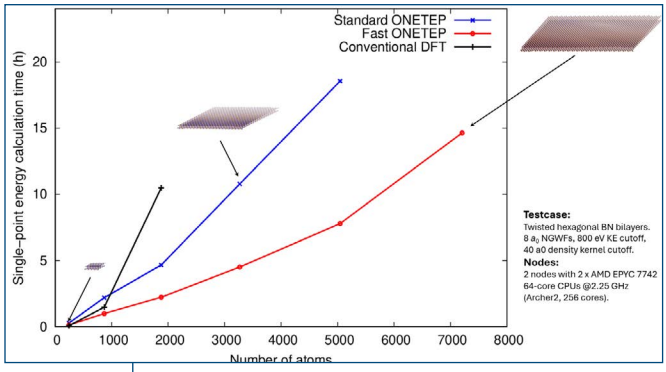


Figure 7: The calculational speed to converge single-point energy for hexagonal BN bilayers with the new fast solver in ONETEP compared to the standard ONETEP solver and CASTEP as conventional DFT solver.

VISUALIZER

Updates to the Materials Studio Visualizer include

- **Materials Studio 2026** supports MaterialScripts in both Perl and Python.
- **Materials Studio 2026** has updated the Perl version, so MaterialsScript is now using Perl 5.40.2.

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

- Use the "Calculate Core Level Spectra" protocol to obtain the absolute position of the core level edge and include spin-orbit splitting of the core level in the calculation of the spectrum.
- "Calculate Hubbard U Values" to refine U values for DFT+U CASTEP calculations.
- Employ "MACE fine tuning" to fine-tune a MACE force field with your data for a particular system. Fig. 8 shows the layout of the protocol.

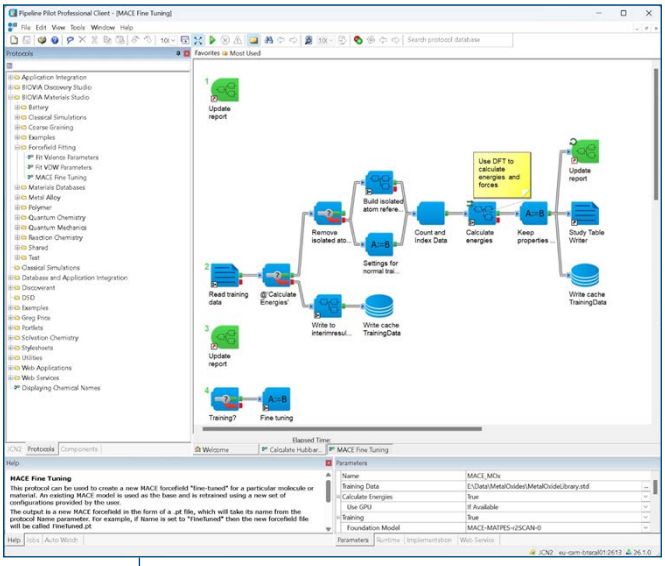


Figure 8: . The new Mace Fine Tuning Protocol in the Pipeline Pilot Materials Studio Collection 2026. This protocol enables to fine-tune a MACE potential by your own data stored in a Study Table.

TUTORIALS

The following new tutorials have been added:

- The **"Building Lipid Membrane in Solvent with Polyethylene"** tutorial teaches how to use the Build Mesoscale Membrane protocol to create a mesoscale bilayer membrane in solution including custom user-defined coarse-grain molecules based on MS Martini 3.
- The **"Modeling of molecular crystals with dispersion corrections"** tutorial demonstrates the use of CASTEP for the modeling of molecular crystals.
- The **"Using Python Scripting to Calculate the Interaction Energy Between Two Layers"** tutorial introduces Python scripting for the Properties Explorer and running Forcite calculations.
- The **"Executing Python Scripts from the User Menu"** tutorial instructs how to use the Script Library to add Python scripts to the User menu in Materials Visualizer.

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