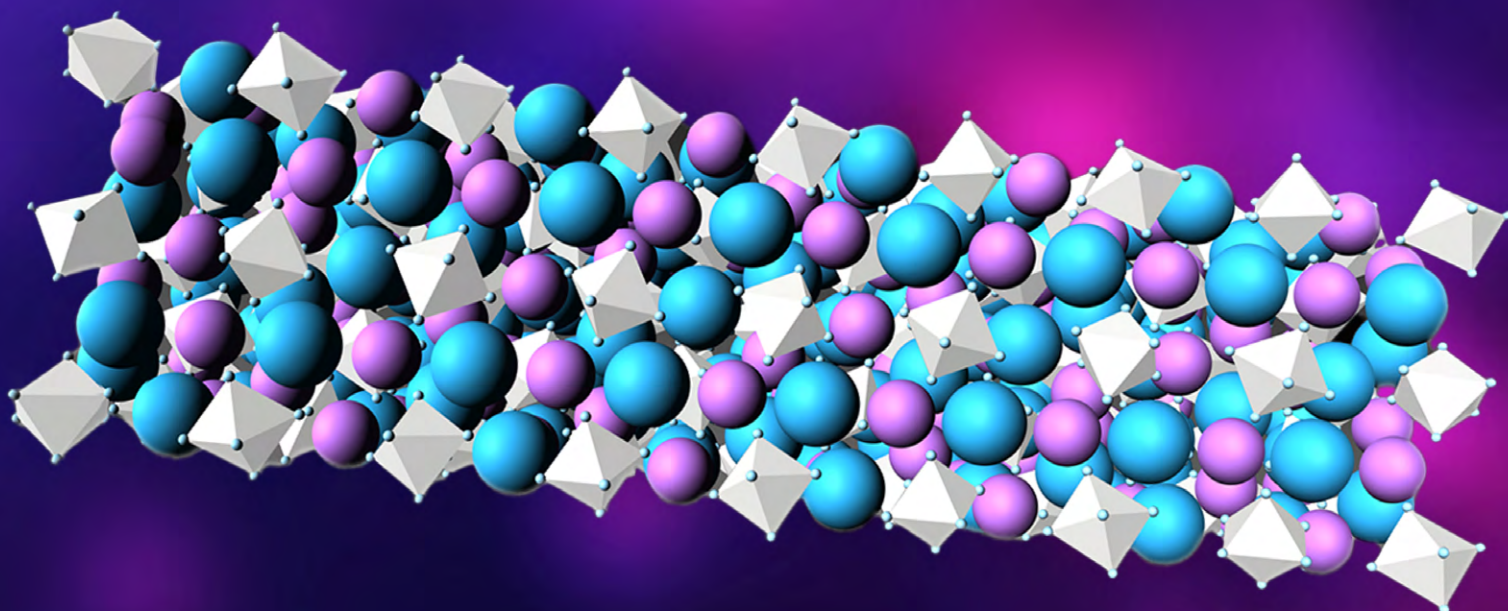


# BIOVIA MATERIALS STUDIO MACE LEARNED FORCEFIELDS

Datasheet



**BIOVIA Materials Studio** MACE Learned Forcefields deliver a powerful combination of accuracy, efficiency, and flexibility for simulating materials, opening up a whole new world of possibilities for modeling chemical phenomena.

## WHAT ARE MACHINE LEARNED FORCEFIELDS?

Machine learned forcefields are an emerging class of tools for running classical simulations that model the interactions between atoms and molecules. Traditional forcefields, such as those based on classical physics principles (e.g., “harmonic valence interactions”) rely on predefined mathematical forms to represent the potential energy of atomic systems. These representations are simplifications that may not capture the full complexity of molecular systems, particularly for materials of unusual composition or chemistry. Additionally, the majority of generalized forcefields do not model chemical reactions between atoms at all.

Machine learned forcefields leverage the power of machine learning (ML) algorithms to create models that predict interatomic interactions directly from data. The training data is based on quantum mechanical calculations (such as density functional theory (DFT) or coupled-cluster methods), which offer a more accurate description of electronic interactions but more computationally expensive than traditional classical forcefields. By using a large training set of quantum data, ML algorithms can generate highly accurate machine learned forcefields that describe the potential energy surface (PES) of molecular systems, thereby improving the predictions of molecular behaviour in simulations. During parameterization, a neural network is trained to map atomic environments to potential energy values and forces, effectively learning how atoms interact within the system. The use of a neural network allows for the flexible representation of the PES, without the need to rely on predefined functional forms for the interactions. The absence of any assumptions about the bonding arrangements of atoms in the molecules also means that chemical bonding changes in reactive systems can in principle be automatically included. This is not possible with traditional forcefields unless parameterised to specific reactions. This new approach promises to significantly speed up the time to solution when investigating new materials without prior knowledge of chemical mechanisms.

## WHY MACE LEARNED FORCEFIELDS?

The use of MACE (Message Passing or Multi-Atomic Cluster Expansion), as with all machine learned based approaches to atomic interaction generation, is motivated by the desire to increase the computational efficiency without compromising on the accuracy of the PES representing the system. MACE uses an extension of the atomic cluster expansion (ACE) approach <sup>[1]</sup> to learn the relationship between the atomic configurations and the PES based on a dataset of quantum mechanical calculations. MACE augments traditional features of graph neural networks to efficiently incorporate high-order features of the local the environment around each atom in a way that allows predictions for systems that may not have been explicitly included in the training dataset <sup>[2][3]</sup>. MACE has emerged as a leading approach with a specific focus on improving transferability.

## FEATURES AND CAPABILITIES

Use the full range of Forcite simulation and analysis tools, along with Materials Studio Visualizer features on the results. Run classical molecular dynamics and evaluate configurational energy using the Forcite module with the following forcefields.

### MACE-OFF23

The foundation of MACE-OFF23 is the SPICE dataset built to replicate forces and energy calculated at the  $\omega$ B97M-D3(BJ)/def2-TZVPPD level of quantum mechanical theory.

You can use MACE-OFF23<sup>[4]</sup> with closed-shell organic molecules. Training data used density functional theory methods for a large set of molecules containing the elements H, C, O, N, P, S, F, Cl, Br, and I.

You can therefore simulate a large variety of materials including biopolymers, drug-like compounds, molecular liquids and crystals.

Highlights include predictions of:

- Sublimation energies comparable with use of DFT with dispersion corrections
- Robust and accurate dihedral scans
- Vibrational and thermal properties of molecular crystals
- Unit cell dimensions within 5%

Three variations of MACE-OFF23 are available with different accuracy levels and cutoffs.

### MACE-MP-0B3

You can use versions of the foundation model MACE-MP0<sup>[3]</sup>, trained on a public database of 150k inorganic crystals- designed to give as complete as possible coverage of the periodic table as possible

- Stable molecular dynamics on wide range of molecules and materials
- Chemical reactions automatically included

### MACE-MATPES-R2SCAN

You can use this foundation model based on a large high quality dataset<sup>[5]</sup> that makes use of the highly regarded r2scan functional.

- Provides improved representation of bonds in material systems

Please refer to original publications for limitations of the listed forcefields.

## KEY FEATURES OF MACE

- **Flexibility:** MACE is versatile and can be applied to a wide range of molecular systems, including organic molecules, inorganic materials, and complex biomolecules.
- **Stability:** Unlike some machine learned forcefield approaches MACE provides very stable molecular dynamics due to the smooth nature of the generated pair potentials between atoms.
- **Transferability:** The model's ability to generalize to new, unseen systems is particularly important when working with novel molecules, materials, or reaction mechanisms.
- **Scalability:** MACE offers computational efficiency, enabling researchers to perform large-scale MD simulations and improved sampling of configurations that would be infeasible with quantum mechanical methods alone.
- **Accuracy:** MACE achieves high accuracy by learning from quantum mechanical data, which allows it to capture more intricate atomic interactions and energy landscapes that classical forcefields cannot describe.
- **Customization:** By starting with an appropriate foundation model such as MACE-MP and adapting the training data highly accurate interactions of specific materials can be built. makes them particularly useful where the specific behaviour of molecules under certain conditions needs to be accurately modelled such as for drug design and catalysis.

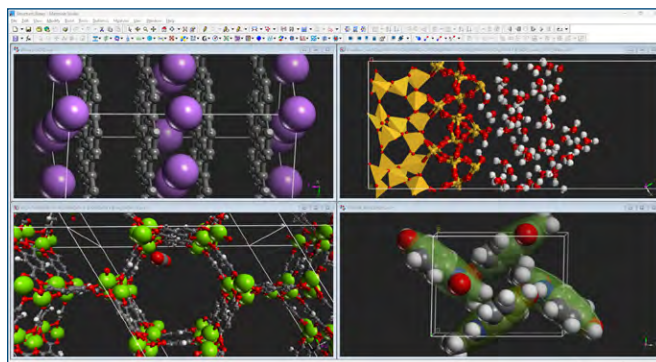
## THE BIOVIA MATERIALS STUDIO ADVANTAGE

The BIOVIA Materials Studio MACE Learned Forcefield module is part of the Materials Studio® software environment. Materials Studio provides a user-friendly interface, complying with Windows standards. Materials Visualizer offers a wide range of model building and visualization tools that allow you to rapidly construct models of the systems of interest.

The MACE Learned Forcefield module is fully integrated with BIOVIA Materials Studio Forcite module and can be used to run molecular dynamics simulations leveraging the range of ensembles, barostats, thermostats and advanced features of Forcite. The BIOVIA Materials Studio CASTEP module is also available within the same Materials Studio® software environment, enabling the generation of new quantum mechanical training data if needed.

The simple user interface, an extensive Help system, and BIOVIA's training programs ensure that even new users will be able to use the program with confidence. A flexible client-server architecture means that calculations can be run on servers located anywhere on your network.

Results are returned to your PC, where they may be displayed and analyzed. You can easily produce high-quality graphics of geometric structures and video clips of molecular dynamics trajectories and which can be imported into other PC applications, assisting you when sharing them with colleagues or when analysing your results using spreadsheets and other packages.



**Figure 1:** Materials Studio MACE Learned Forcefields can simulate a diverse range of materials models to provide insights and property predictions.

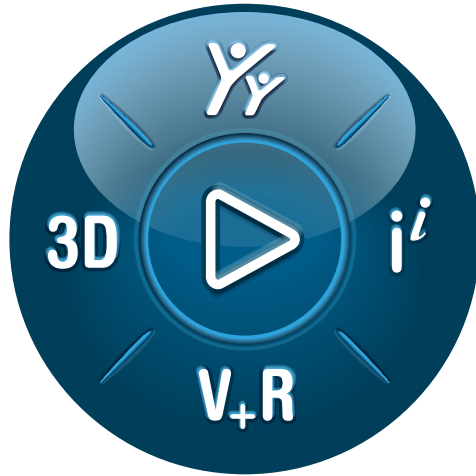
MACE represents a significant advancement in the field of machine-learned forcefields by providing smooth, accurate and transferable models of molecular interactions. With its ability to replicate quantum-level accuracy at a much lower computational cost, MACE is a powerful tool for materials science, and the study of complex biochemical systems.

LEARN MORE

To search the many application examples, see this [list](#)

## REFERENCES

1. R. Drautz, "Atomic cluster expansion for accurate and transferable interatomic potentials," Phys. Rev.B, vol. 99, p. 014104, Jan **2019**.
2. Batatia, I. et al "MACE: Higher Order Equivariant Message Passing Neural Networks for Fast and Accurate Force Fields", Advances in Neural Information Processing Systems, 11423-11436 (**2023**).
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4. Kovács, D. P. et al "MACE-OFF23: Transferable Machine Learning Force Fields for Organic Molecules" <https://arxiv.org/abs/2312.15211> (**2023**).
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