

Parametrization

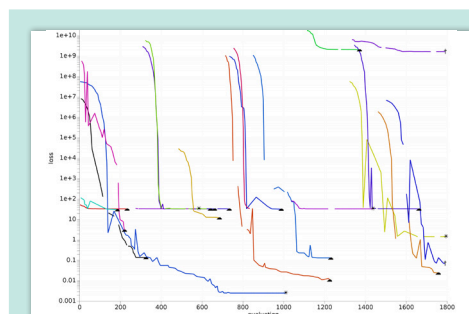
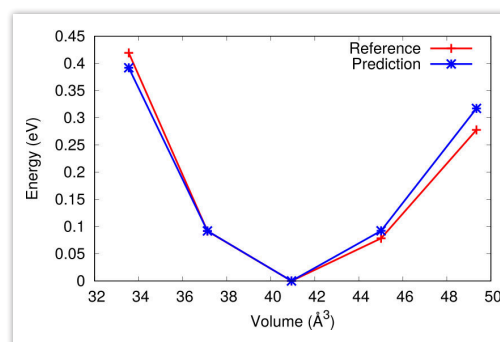
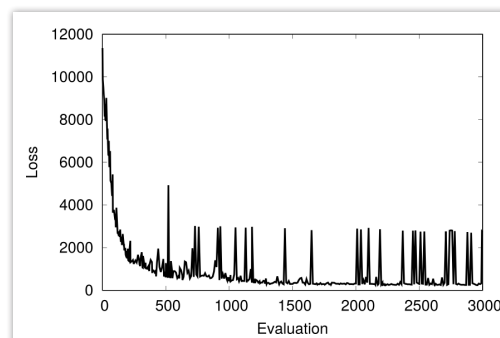
with the Amsterdam Modeling Suite

Create custom models or fine-tune existing ones for your research

Atomistic modeling can help reduce time and wasteful experiments by suggesting the best materials out of millions of candidates. Interatomic potentials are fundamental to perform atomistic simulations beyond quantum mechanics. However, the parameters might be unavailable or unsuitable for your application. With ParAMS, you can create your own models to describe novel materials and molecules.

What can you do with ParAMS?

- Optimize ReaxFF, DFTB, and Machine Learning Potentials (MLP) parameters
- Tune parameters to describe properties such as energies and forces, reaction energies, geometries, stress tensors, charges, band structure, etc.
- Use single points, geometry optimizations, or PES scans during the parametrization
- Optimize and fine-tune M3GNet

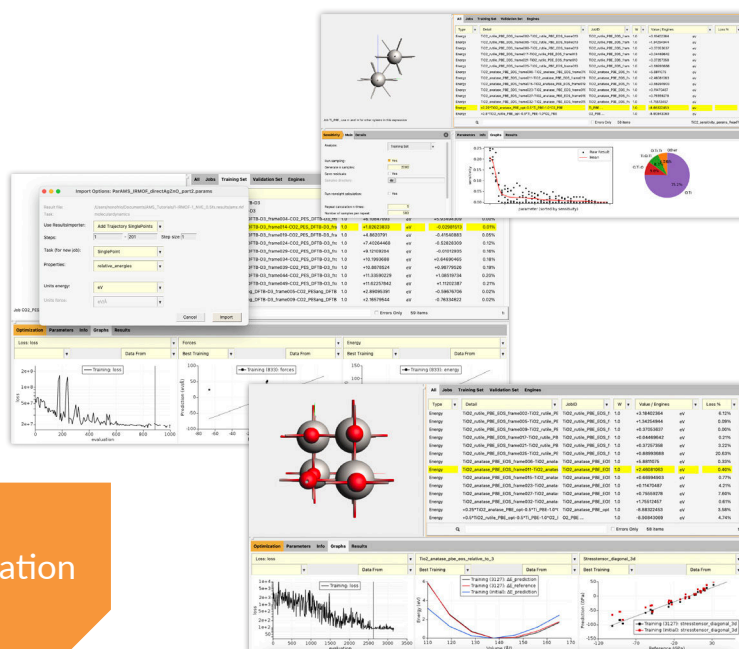


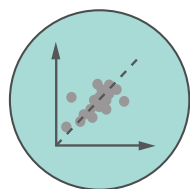
Key features of ParAMS

- ✓ Import reference data from AMS, VASP, QE, Gaussian, or experiments
- ✓ Use training and validation sets to prevent overfitting
- ✓ Submit multiple optimizations in parallel, interactively stop and restart
- ✓ Explore the sensitivity of the parameters (ReaxFF and DFTB)

A dedicated graphical user interface for ParAMS

- Import structures and visualize the dataset
- Interactively display the optimization results (loss, energy and force parity plots)
- Select and inspect outliers
- Submit jobs to a remote machine





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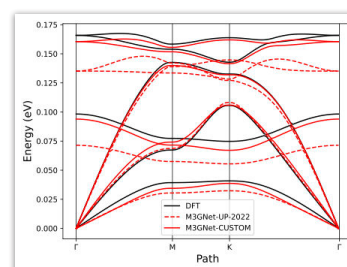
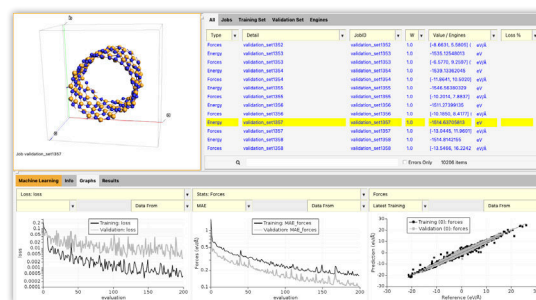
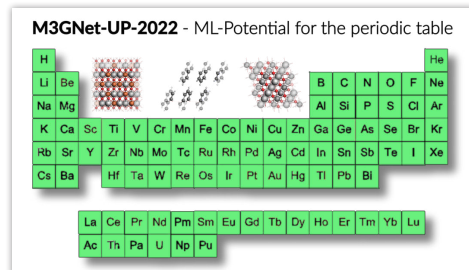


Active learning

The active learning workflow is used for on-the-fly training of MLP during molecular dynamics. The workflow consists in training an initial MLP, running the MD simulation, launching new reference calculations at set intervals. If the MLP is not accurate enough, it is retrained to the new reference data. Then the MD simulation is taken to the last point where it was known to be accurate and continued. This results in an automatic framework to develop dedicated MLP to perform an MD task.

Fine-tuning M3GNet

M3GNet is a graph neural network potential that was recently proposed. One of the novelties of M3GNet is that it was trained over a large database of crystal structures, resulting in a universal potential (e.g. covering most of the elements in the periodic table). However, the model might not be accurate enough for your system, and you might want to re-optimize it from scratch, or locally. Here we show the performance of the original M3GNet model to describe monolayer hexagonal boron nitride compared to a custom version of M3GNet that was re-optimized against a large dataset of BN structures.



“What I really like about the Amsterdam Modeling Suite is that the programs were clearly written by chemists for dealing with real chemical problems. A great suite of programs!”

– Roald Hoffmann, Nobel Laureate

About SCM

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