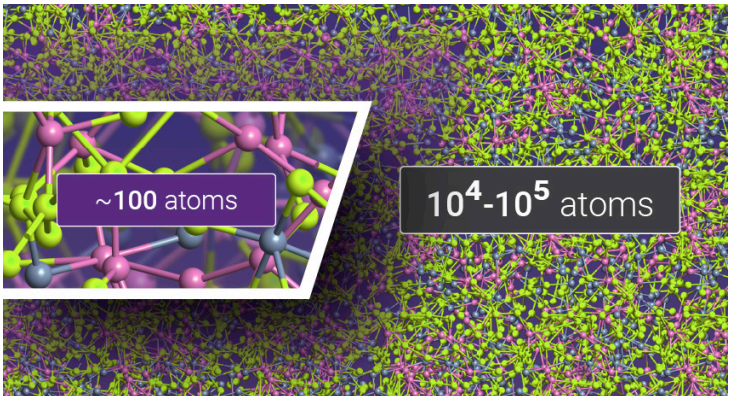
SYNOPSYS®

# Machine-Learned Force Fields with QuantumATK

**Machine-Learned Force Fields (ML FFs)** provide near-*ab initio* accuracy for large realistic system sizes and dynamical simulation time-scales greatly exceeding those accessible to Density Functional Theory (DFT). Use ML FFs in QuantumATK to generate realistic complex structures of novel crystal and amorphous materials, alloys, interfaces, and multilayer stacks, simulate thermal and mechanical properties, diffusion and surface processes. Benefit from the pre-trained ML FF library or develop new ML FFs using automated and efficient training and simulation workflows. Employ ML FFs for molecular dynamics (MD), force bias Monte Carlo, nudged elastic band (NEB), and geometry optimization simulations.

## ML FFs for Dynamical Simulations of Large-Scale Realistic Systems

- **1000 to 10,000x faster than DFT**, thus enabling dynamical modeling of realistic novel and complex systems containing even 100,000+ atoms, instead of small model 100-atom systems.
- **Provide near-*ab initio* accuracy** for multi-element materials, heterogeneous systems like interfaces, and systems far from equilibrium, including amorphous materials, phase transitions, or chemical reactions.
- **Often easier to develop than conventional FFs** using the automated workflows available in QuantumATK. Accurate conventional FFs for such complex materials would require much more extensive and complicated development processes.




## Automated Efficient Generation of ML FFs

### Automatic Workflows

**Basic workflow**
- For crystalline materials
- Automatically generate training configurations, compute training data with DFT, and perform machine learning, i.e., fitting to the training data

**Advanced active learning workflow**
- For amorphous systems, interfaces, systems at high T, surface processes
- Improve initial ML FFs generated with the basic workflow by actively adding training configurations and DFT training data during MD simulations

### Templates & GUI

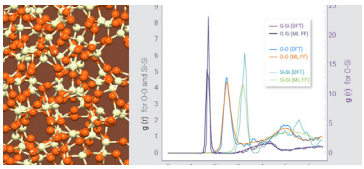
- Use automatic training tools and GUI templates [1,2] for:
  - crystal & amorphous bulk materials
  - interfaces
  - molecules
- Inspect automatically generated training configurations using GUI
- Validate generated ML FFs by comparing calculated values with available experimental and DFT data:
  - RDF and ADF
  - Elastic constants
  - Neutron scattering factor
  - Chemical composition profile
  - X-ray scattering

### QuantumATK Advantages

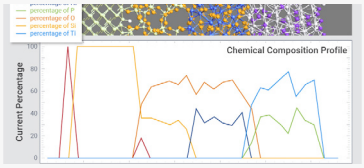
- Automated user-friendly generation of training data, tailored for specific applications
  - Ensures minimal amount of training data and time needed
  - No computationally expensive *ab-initio* MD is needed in most cases
  - Provides good quality accurate ML FFs for complex systems
- Single interface for different simulation engines
  - Easily switch between training with DFT-LCAO and DFT-PW
  - Combine ML FFs with conventional FFs, DFT or Semi-empirical calculators


www.synopsys.com/silicon/quantumatk/atomistic-simulation-products/machine-learned-force-fields.html

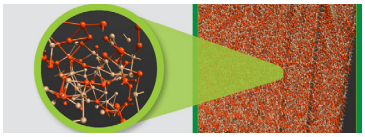
# Application Examples of Machine-Learned Force Fields



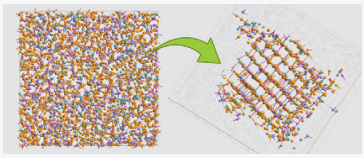
**Structure Generation of Amorphous Materials:** Generate amorphous structures for PCRAM, ReRAM and FeRAM novel memories, solar cell and other applications. In this example, 80 ps ML FF - MD generated am-$SiO_2$ structure of 600 atoms in 11 minutes, whereas it took 10 days to generate 72-atom structure with DFT-MD on 16 cores. Structural parameters obtained with ML FFs are in a good agreement with DFT and experimental results.



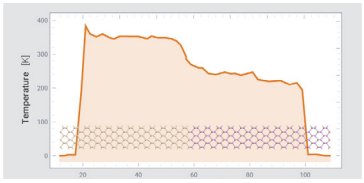

**Structure Generation of Interfaces and Multilayer Stacks:** Build and optimize complex crystalline and amorphous interfaces and multilayer stack structures for semiconductor development applications, such as high-k metal gate (HKMG) (using Multilayer builder GUI) and MRAM magnetic tunnel junction engineering. This example shows a generated structure of nearly defect-free c-Si|am-$SiO_2$|am-$HfO_2$|am-$Ti_2N$ HKMG stack.



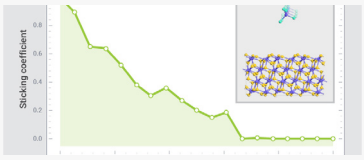
**Structure Generation of Glassy Amorphous Materials:** Generate glassy amorphous materials with impurities for optoelectronic applications. In this example, ML FF – MD is used to simulate a large- scale 120,000 atom size sodium silicate glass with Na impurities, $(Na_2O)_2(SiO_2)_{40000}$ at 2500 K.



**Crystallization & Amorphization Processes:** Study *ns*-long crystallization and amorphization processes with ML FF - MD in large-scale systems for, e.g., PCRAM novel memory applications. This example depicts crystallization of 2520-atom phase change alloy material $Ge_2Sb_2Te_5$.




**Thermal Property Simulations**: Simulate thermal conductance using ML FFs with *ns*-long reverse non-equilibrium MD (RNEMD) simulations for developing PCRAM and evaluating self-heating and heat dissipation in devices. Examples include simulating thermal conductance in bulk $Ge_2Sb_2Te_5$ (2300 atoms), $Ge_2Sb_2Te_5$/Si (882 atoms) and Si/GaAs (864 atoms) interfaces, monolayer $MoS_2$ (108,000 atoms). Calculated values are in a good agreement with experimental and DFT results where available.




**Surface Process Modeling:** Simulate thermal ALD and ALE processes using specifically trained ML FFs with MD. This example shows simulation of thermal ALD process: $HfCl_4$ deposition on $HfO_2$ surface of 4.5 $nm^2$ area. Precursor adsorption energies are consistent with DFT results. Obtained sticking coefficient and coverage values can be used as parameters for feature scale models to optimize yield of ALD.

# Built-in Library of Ready-to-Use Machine-Learned Force Fields

- QuantumATK offers Moment Tensor Potentials (MTPs) ML FFs implemented by the QuantumATK team in-house.
- MTPs provide high robust accuracy with lower computational cost compared to other ML FFs [3,4].
- Benefit from the pre-trained ready-to-use high-quality MTP library [5,6] or develop MTPs for new materials, interfaces and surface processes by using automatic generation workflows.


Bulk crystal and amorphous

Crystal/amorphous and amorphous/amorphous interfaces

Surface process simulations


Tutorial and video on automatic ML FF training tools and GUI templates

[1] Tutorial: https://docs.quantumatk.com/tutorials/mtp_hfo2/mtp_hfo2.html [2] Video: https://www.youtube.com/watch?v=6BrrVotzjnc

[3] A. V. Shapeev. *Moment tensor potentials: a class of systematically improvable interatomic potentials.* Multiscale Model. & Simul. **14**, 1153 (2016).

[4] Y. Zuo, C. Chen, X. Li, Z. Deng, Y. Chen, J. Behler, G. Csányi, A. V. Shapeev, A. P. Thompson, M. A. Wood, and S. Ping Ong. *Performance and cost assessment of machine learning interatomic potentials.* J. Phys. Chem. A **124**, 731(2020).

[5] ML FF features: https://www.synopsys.com/silicon/quantumatk/resources/feature-list.html#MLforcefield

[6] Materials in ML FF library: https://docs.quantumatk.com/manual/ForceField.html#pretrained-moment-tensor-potential-mtp-parameter-sets



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