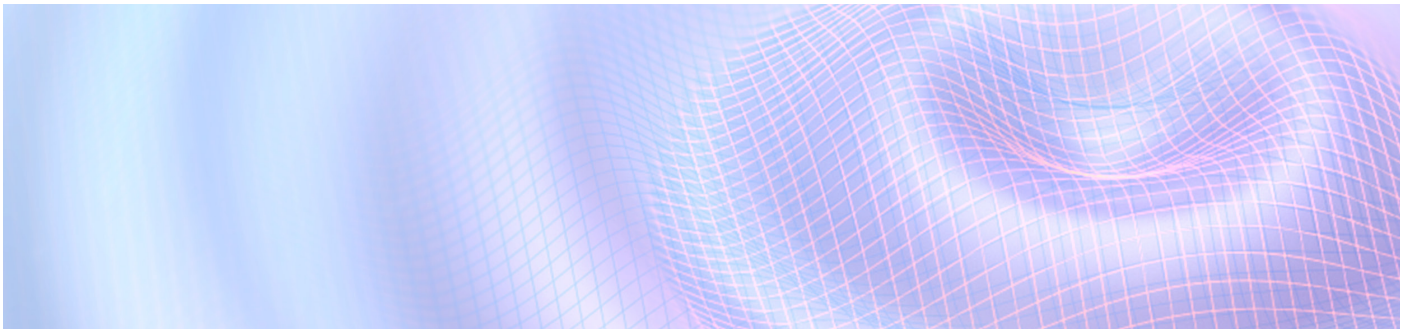
SYNOPSYS®

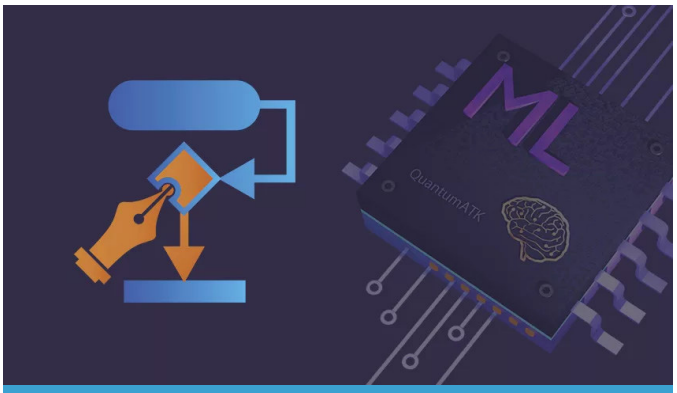
QuantumATK Release Features

Last amended: December 2023

QuantumATK V-2023.09

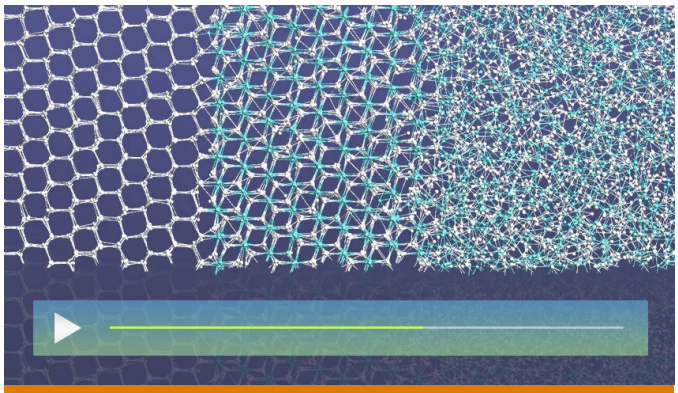
QuantumATK is a leading industry-proven platform for atomic-scale modeling of materials, nanostructures, and nanoelectronic devices. It includes quantum mechanical methods such as density functional theory (DFT) with either LCAO or plane-wave basis sets and semi-empirical models, simulation engine for atomic-scale simulations using classical potentials, module for nanoscale device and transport simulations using non-equilibrium Green's function (NEGF) methodology. QuantumATK combines the power of a Python scripting engine with the ease-of-use provided by an intuitive graphical user interface, NanoLab. All simulation engines share a common infrastructure for analysis, ion dynamics and parallel performance techniques.





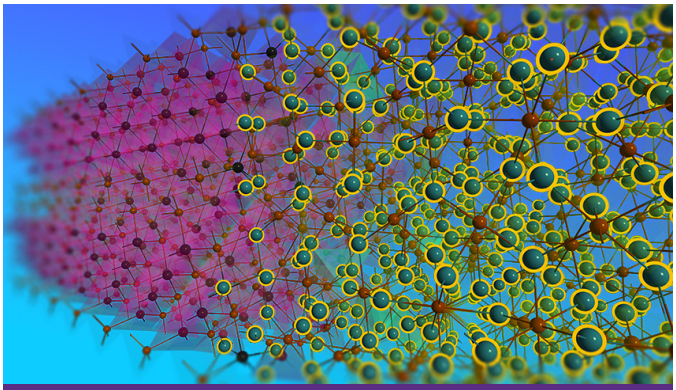
Machine-Learned Force Field Training

- Enhanced ease-of-use of training ML FFs with new predefined Workflow Builder blocks for active learning simulations and training sets.
- New ML-FF training template for defect structures.



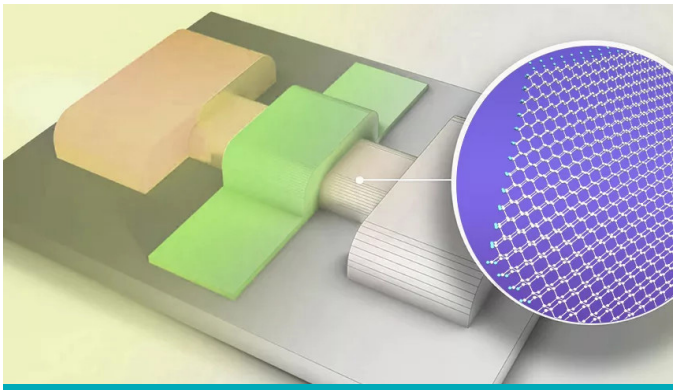
Process Simulations

- Accelerated molecular dynamics for crystallization.
- Thermochemistry pyrolysis to predict gas phase composition in surface processing.
- Integrated workflow and analysis of charged point defects and defect diffusion.



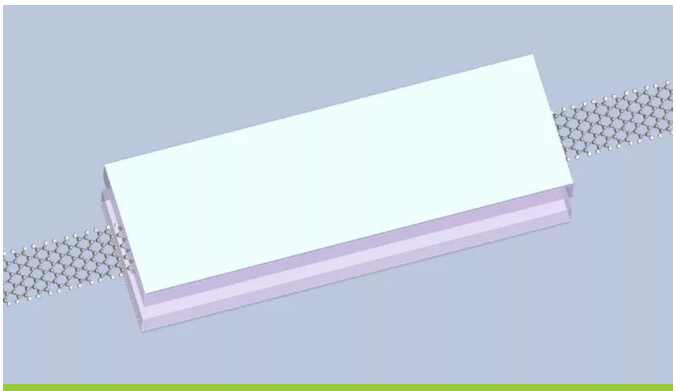
Interface Modeling

- New interactive Interfaces Builder for multilayer structures.
- High-k Metal Gate (HKMG) and Magnetoresistive RAM (MRAM) Builders as Workflow Builder blocks can be part of simulation workflows.
- New Projected Phonon DOS analysis.



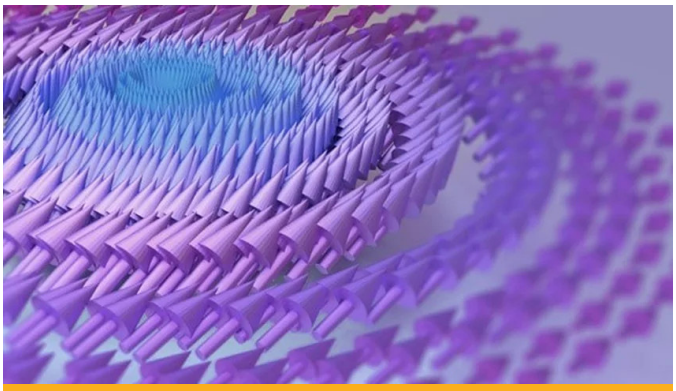
Device Channel Material Design

- Major speedup in bandstructure simulations with Semi-Empirical Tight-Binding models for up to million atoms.
- Efficient and simplified deformation potential extraction for large nanostructures to evaluate electron-phonon coupling.



Nanodevice Modeling

- New analysis of spectral and thermal current and conductance in Transmission Analyzer.
- More interactive IV Characteristics Analyzer and possibility to analyze inelastic current.



STT-MRAM Memory Design

- New Finite Bias Spin Transfer Torque (STT) Study Object and Analyzer to evaluate the write performance of STT-MRAM.
- New Heisenberg Exchange Analyzer for exchange couplings and Curie temperature.

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