SYNOPSYS®

QuantumATK Release Features

Version P-2019.03

Last amended: November 2019

QuantumATK P-2019.03

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.

DFT Updates

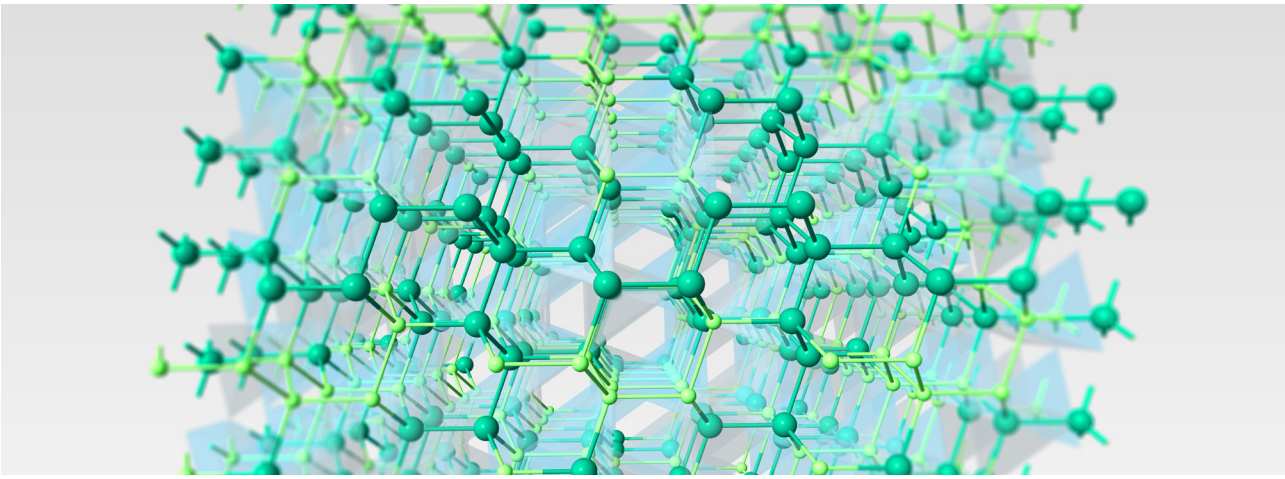
- Employ the **SCAN MetaGGA functional** in both LCAO and plane-wave calculations for significant improvements over GGA and LDA in many different systems
- Speed up your plane-wave simulations by using the **Projector-Augmented Wave (PAW) method** (beta version)
- Discover **new analysis objects for plane-wave calculations**, such as optical spectrum, effective band structure, fat band structure, and projected density of states
- Use the Kerker preconditioner to improve convergence for slab calculations when using plane waves
- Run hybrid HSE non-collinear and non-collinear spin-orbit calculations
- Enjoy significant performance improvements in HSE calculations by using a reduced exchange grid without noticeable loss of accuracy (new default), and by reusing the wavefunctions for density of states (DOS) analysis
- Take advantage of the added GGA PseudoDojo normconserving pseudopotentials with support for noncollinear spin-orbit interaction

Analysis Objects Updates

- Perform **magnetic anisotropy energy** calculations using a versatile study object with smart restarting and a flexible analysis framework
- Calculate **partial electron density** and visualize it in real space, e.g., show a cut plane above a surface which corresponds to a simulated STM image within the Tersoff-Hamann approximation
- Obtain a **surface band structure**, which is a device density of states evaluated along a k-point route perpendicular to the surface or transport direction
- Perform improved **effective band structure** analysis calculations, with no constraints on defect location, element, defect type, etc.

Dynamics Updates

- Explore the **time-stamped force-bias Monte Carlo** method, coupled to DFT, DFTB or force fields, as an alternative to molecular dynamics for long time-scale equilibration, deposition, amorphization, diffusion, sampling of rare events, etc., either at constant temperature or with a linear heating/cooling ramp
- Note the significantly faster runtime and improved parallel scaling of HamiltonianDerivatives and DynamicalMatrix calculations, thanks to the use of symmetries to reduce the number of displacements (also, the k-point sampling is now automatically scaled with the supercell size)
- Choose the newly added **Brenner/REBO** and **Moliere** potentials in etching and deposition simulations
- Save time by being able to restart relaxation of devices from partially optimized device configurations
- Constrain the space group in geometry optimizations of crystalline materials



Performance Improvements

- Enjoy significant memory and calculation time reductions for **DFT LCAO molecular dynamics (MD) and geometry optimizations**, to the point where one can now comfortably run these calculations with several hundred or even thousands of atoms
- Benefit from general performance improvements in DFT MGGA, GGA, Hybrid, and non-equilibrium Green's function (NEGF) calculations
- Employ **MPI parallelization of force-field potentials** to speed up large-scale MD simulations
- Parallelize Green's function inversion over multiple processes per contour point for reduced memory footprint
- Use the new ParallelDevicePerformanceProfile function to get advice on the best parallelization strategy (memory and speed) for NEGF calculations
- Improved performance in the GUI (LabFloor load time, NEB generation, etc.)

More Customizable Script Generator

- Enjoy a reorganized **script board** with better user experience
- Use the new layout for **calculator widgets** to focus on the most important parameters
- Save your calculator settings and workflows as **templates** and reuse them in future calculations

Enhanced 2D Plot Framework

- Perform **advanced editing** of plots, save them for further analysis, and reuse plot setups with new data
- **Link and combine** various plots for more insightful analysis
- **Fit data** to linear and other models and measure directly in graphs

Miscellaneous Updates

- **Symmetrize crystal structures** in the Builder based on approximate space groups, and change angle and position tolerances in crystal symmetry detection
- Take advantage of newly included packages: Pandas and Fireworks
- Experience the benefits of **Python 3**, which QuantumATK is now based on

Downloading and Installing QuantumATK P-2019.03

Get QuantumATK P-2019.03

If you are a customer entitled to maintenance services, you can access QuantumATK P-2019.03 and download release and installation notes directly from SolvNet .

Download QuantumATK P-2019.03 & Release Notes

Licensing Updates

To run QuantumATK P-2019.03, customer must:

1. Use the Synopsys Common Licensing (SCL) software, version 2018.06 or later, and
2. Have a license key files generated on December 10, 2018 or later

Updated license key files and the latest version of SCL can be downloaded from your account on SolvNet.

Synopsys QuantumATK Team
Fruebjergvej 3
DK-2100 Copenhagen
DENMARK
Tel: +45 333 32 300
Email: quantumatk@synopsys.com