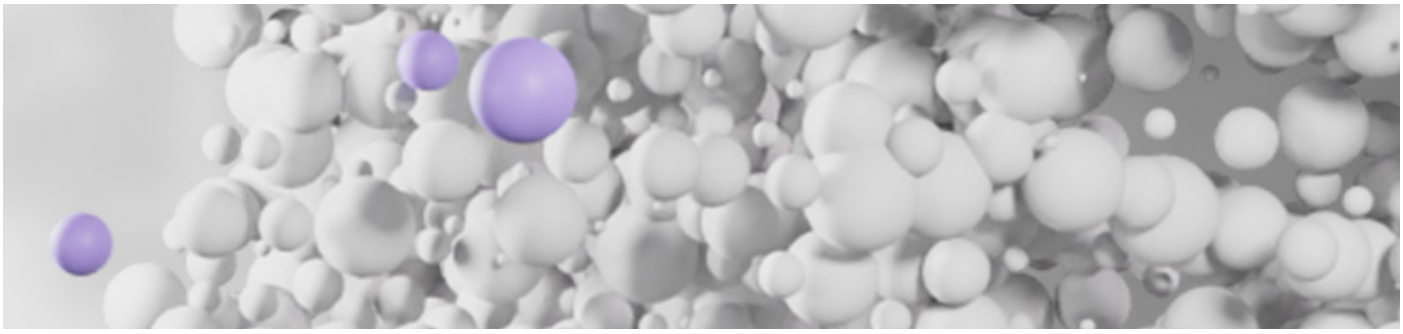
SYNOPSYS®

QuantumATK Release Features

Last amended: December 2022

QuantumATK U-2022.12

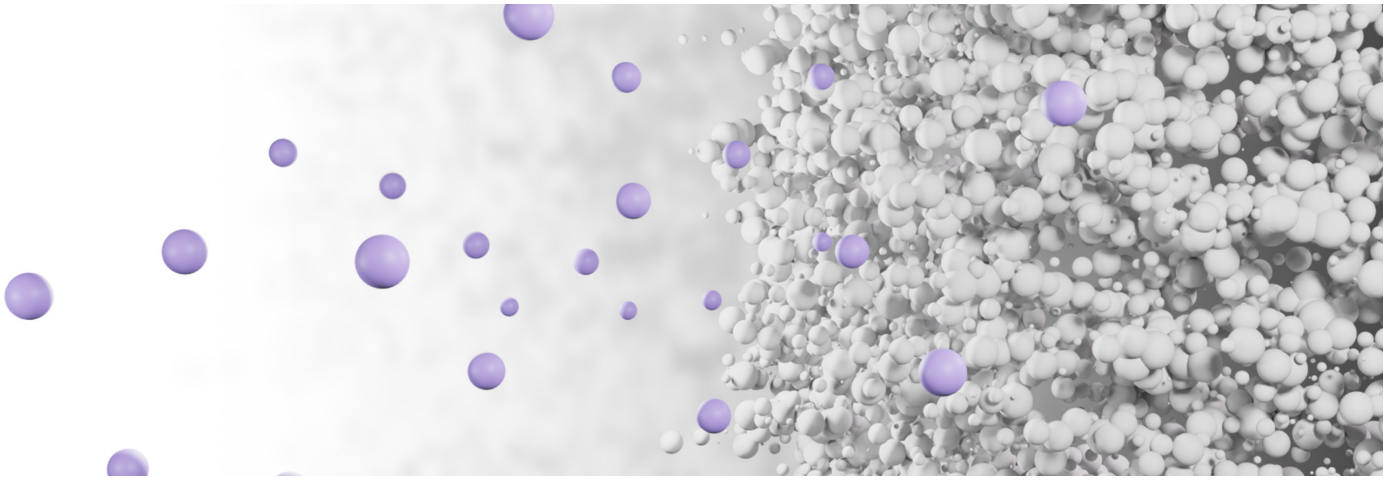
QuantumATK is a leading industry-proven platform for atomic-scale modeling of materials, nanostructures, and nanoelectronic devices. It includes quantum mechanical methods such as density functional theory (DFT) with either LCAO or plane-wave basis sets and semi-empirical models, simulation engine for 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.



Downloading and Installing QuantumATK U-2022.12

Download

If you are a customer entitled to maintenance services, you can access QuantumATK U-2022.12 and download full release and installation notes directly from SolvNetPlus: https://solvnetplus.synopsys.com.



New Features in QuantumATK U-2022.12

Machine-Learned (ML) Force Fields & Thermal Properties

In this release, we have continued to develop our ML force field framework using Moment Tensor Potentials (MTPs). 1000-10,000x shorter computational time vs DFT enables ab initio accuracy for large system sizes and time scales greatly exceeding those accessible to DFT.

- Available MTP library with pre-trained MTPs for a range of bulk materials and interfaces.

Updates to the Core MTP Framework

- Significantly improved accuracy for multi-element systems using more a flexible design of the potential coefficients.
- New extrapolation grade algorithm for active learning: Query-by-Committee.
- The most important MTP training workflows are now accessible in the new Workflow Builder in the Nanolab GUI for fast and easy setup.
- Built-in MTP analyzer to plot correlation between MTP and reference DFT energy, forces, and stress from Data Tool in Nanolab.
- Training protocol updates (generating training data for alloy materials and improvements for interface training protocol).
- Improvements to MTP training functionality.
- CrystalPropertyValidation analysis object.

Pretrained MTP library

- New pre-trained MTP models.
- Re-trained MTP models for HKMG stack and interfaces, with added gate metals Ru, Sc, and their interface with HfO_2.
- Re-trained TiNAlO potential with improved accuracy.

Multilayer Stack Generation using the Multilayer Builder GUI

- New MTJ builder to build stack configurations for magnetic RAM (MRAM) applications.
- Improvements in features and quality of the generated structures from the HKMG builder.
- General multilayer builder improvements, specifying displacement vectors for better aligning of crystal interfaces.
- Tutorials to explain how to build HKMG and MRAM stacks.

Defect-Assisted Recombination from DFT Calculations

- Support calculations of Shockley-Read-Hall (SRH) capture rates. SRH calculations are supported for LCAO and PlaneWave calculators, for both LDA/GGA functionals and hybrid HSE.
- Compute luminescence line shapes for color centers, which can be used for defect characterization by modelling photoemission experiments.
- Dedicated SRH Analyzer makes it easy to perform advanced analysis and drill down deeper into the results, and e.g., inspect the individual electron-phonon coupling contributions.

Modelling of Homogeneous Electric Fields in DFT

- Updates to electric fields implementation in periodic calculations (integrated and extended feature in terms of applicability).
- The model accounts for the effects of field-driven electric enthalpy, forces, and stresses via the Berry-phase polarization theory.
- Supported for LCAO and Plane-Wave.
- Suitable for insulators and semiconductors (metals are not supported).
- Provides a TAT/QoR trade off control: recalculation of Polarization and Born Effective.
- Charge along trajectories can be tuned from “frozen” to continuously updated.
- Performance improvements for Polarization and Born Effective Charge calculations and additional performance can be gained by using the newly enabled multilevel parallelism.

Atomistic Spin Dynamics - Integration with Vampire

- Vampire (atomistic magnetic simulation code) is integrated into workflows that enable studying spin dynamics and stability of the magnetic free layer in magnetic tunnel junctions for MRAM technology.
- This workflow is an ideal combination of simulation methods:
  - DFT-based input to spin dynamics calculations.
  - Use ML-fitted force fields to obtain more than 1,000x faster geometries with the same accuracy.
  - Vampire can compute a wide variety of properties with atomic resolution for realistic system sizes (5,000+ atoms).
- Set up the full DFT-to-Vampire simulation flow in the NanoLab GUI, which automatically builds the required script to compute the required input parameters Heisenberg exchange constants and magnetic anisotropy energy.
- Launch the Vampire calculation from a QuantumATK Python script via wrapper classes (works both on Windows and Linux).
- Visualize Vampire output Curie temperature, anisotropy energy, and hysteresis curves can be visualized and analyzed using dedicated plotting tools in the GUI.
- One can study STT-MRAM & SOT-MRAM, switching time & mode, temperature dependence, skyrmions, 2D magnetic materials and much more. More information can be found in Vampire website.

R2SCAN Exchange-Correlation Functional

- The recently developed r2SCAN meta-GGA functional is now available in QuantumATK and can be simply selected in the GUI Scripter.
- r2SCAN maintains the numerical performance that rSCAN provides over SCAN, but unlike rSCAN it satisfies the exact constraints that the exchange-correlation should obey.

PAW method for LCAO (Beta Version)

- LCAO-DFT calculations can now also make use of the PAW (Projector Augmented Wave) method, as has been possible with PlaneWave-DFT for some time. Note that in the U-2022.12 release, not all analysis options are yet available for LCAO-PAW, support is limited to bulk and molecule configurations, and only GGA functionals can be used.
- Optimized basis sets are available for Fast and Accurate calculations.

COSMO and COSMO-RS

A major new feature in this release is the inclusion of COSMO (COnductor-like Screening MOdel) to study solvation effects, as well as COSMO-RS to evaluate solubility and a range of other properties.

- The calculations can be performed with the solvent either as a perfect conductor or as a dielectric corresponding to a particular solvent.
- Setting up COSMO calculations is automated in the new Workflow Builder and is added as an option in LCAO-DFT calculations for molecule and bulk configurations, and Device LCAO-DFT for surface configurations.
- Non-electrostatic effects such as dispersion and cavitation energies are estimated with a linear regression model.
- Solvation free energies, including non-electrostatic and gas phase terms can be automatically calculated.
- The COSMO solvent surface can be visualized in the Viewer, showing the solvent cavity shape and the charge polarization across the surface.

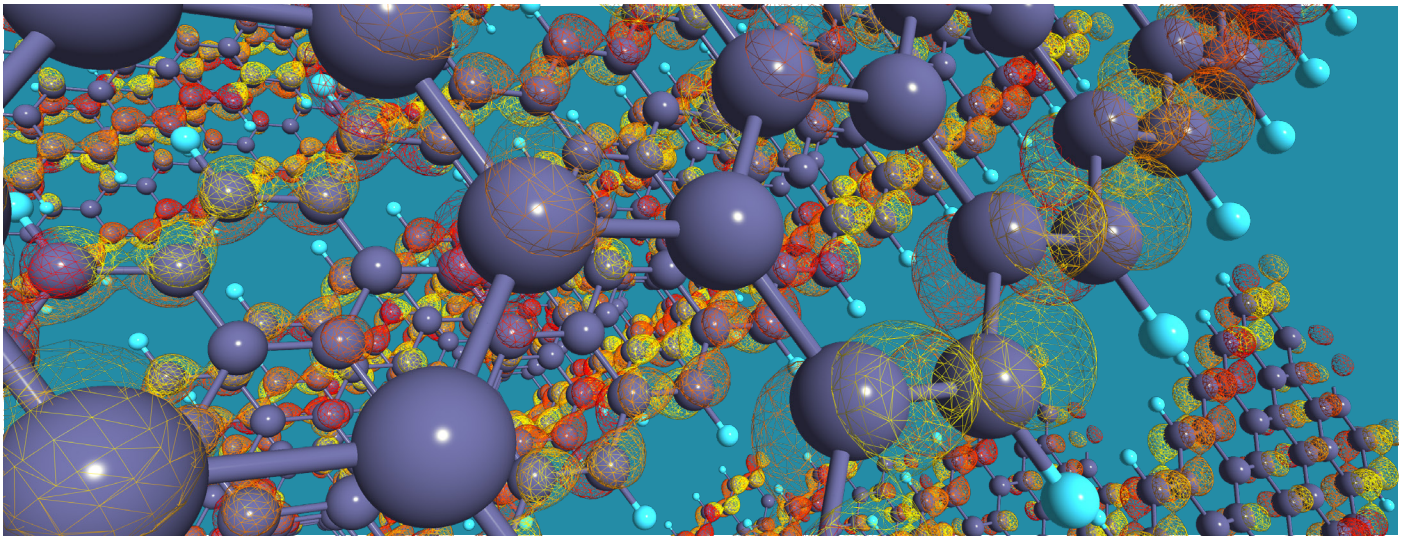
COSMO-RS is an extension of the COSMO model that uses the surface charges generated in the COSMO calculation to calculate the chemical potential of a molecule. GUI-features of the COSMO-RS Analyzer include:

- Calculations of different properties can be set up easily, including investigating the effects of temperature or different solvent composition.
- Results are shown graphically and in text format.
- The sigma profile and potential for molecules can also be displayed.
- The analyzer includes a database of approximately 1,500 molecules that can be added to a COSMO-RS calculation.
- New molecules can be added to the database through a simple drag and drop interface. The appropriate DFT calculations for each molecule can be automatically set up in the Workflow Builder.
- The parameters of the COSMO-RS method are editable in the COSMO-RS Analyzer. Some pre-defined parameter sets can be selected, or a user-defined parameter set can be used. Parameter sets can also be saved for later use.

New Workflow Builder

The Workflow Builder (watch video) is a tool to set up complex workflows which can involve several separate simulations which are later used as input for various post-processing calculations. Here is a list of noteworthy features:

- When editing Workflow Blocks, non-default values are clearly indicated, and there is a function for direct “reset” to defaults
- All modified Workflow Blocks can be saved in the “Blocks” catalog for easy reuse in other workflows
- Workflow Blocks can be grouped together in a container block called the “Block of Blocks”. Since a Block of Blocks can be saved, this allows for the re-use of even very complex calculation setups
- The Workflow Builder supports the inclusion of already calculated results through the “Load Block”. All QuantumATK objects can be loaded and used directly within a workflow. The obvious example is the calculation of additional analyses from an already updated configuration
- When exporting to the script, the Workflow Builder allows for specifying both filename and object id



Updates Related to Molecular Dynamics and Force Fields

Surface Process Simulations

- Adaptive thermostat height enables efficient substrate thermalization even for thick layer growth.

Polymer Simulations

- Apply bead definitions to an all-atom structure to automatically convert it to a coarse-grain representation.

Ion Dynamics

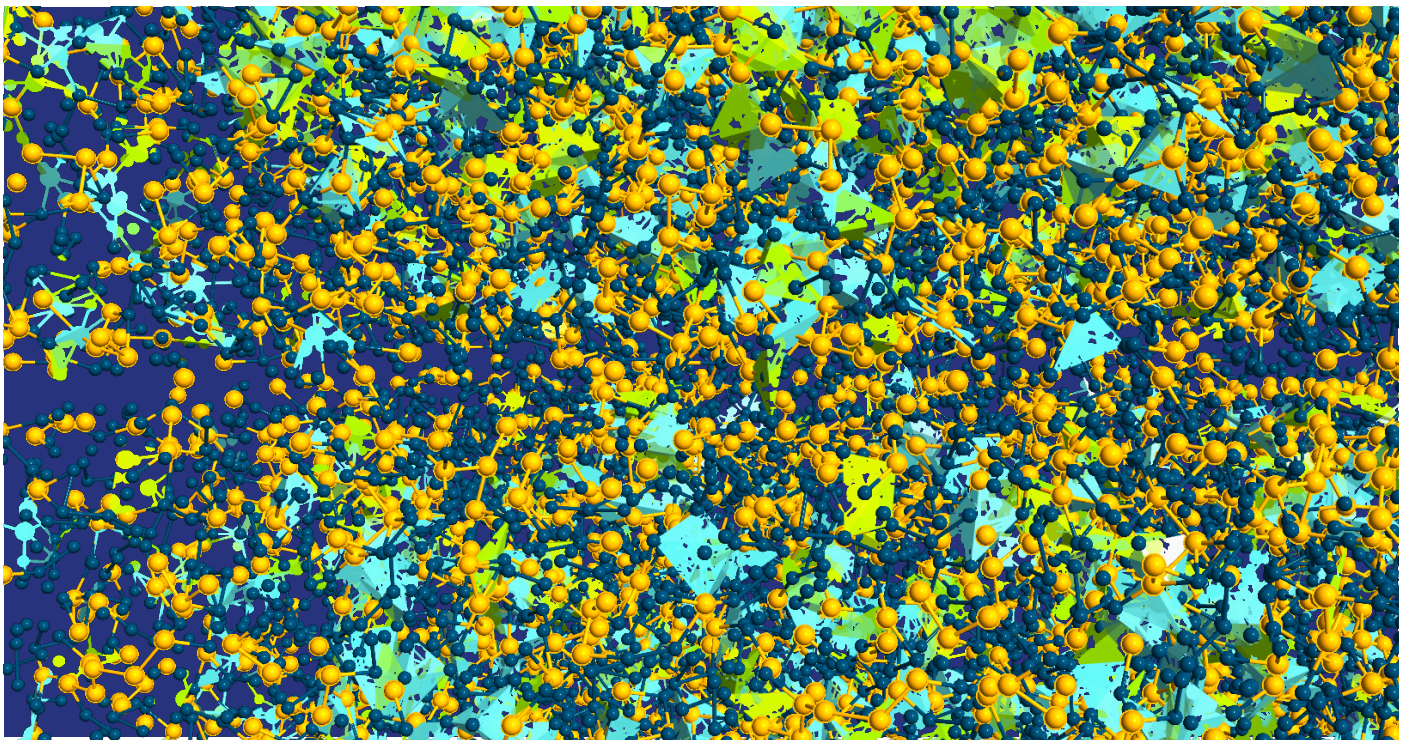
- New state-of-the-art NVT thermostat (Bussi-Donadio-Parrinello stochastic velocity rescaling) which combines the advantages of the Berendsen and Nose-Hoover thermostats.
- Added option to save raw (i.e., unconstrained) forces and stress in optimization trajectories to be able to use it for MTP training.
- The confusing parameter “disable_stress” in OptimizeGeometry has been replaced by “optimize_cell”.

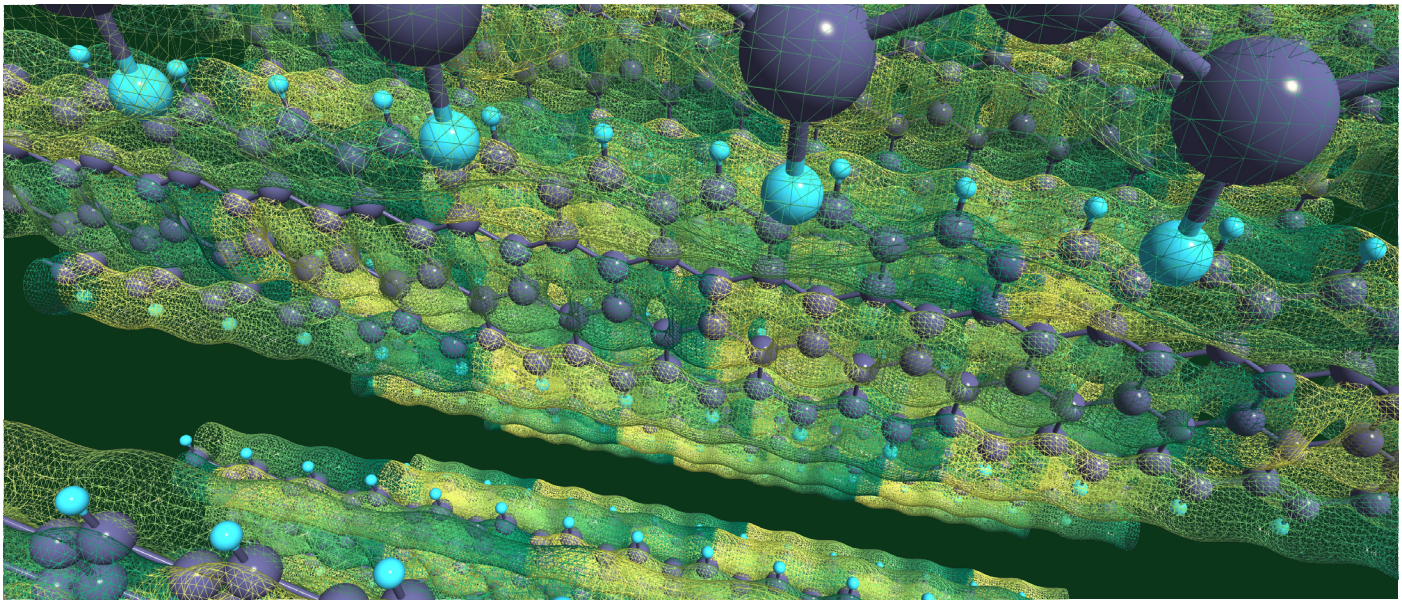
Force Fields

- Included state-of-the-art methods for charge equilibration, e.g., D4-EEQ, which is based on the Grimme-D4 scheme.
- New force fields for various glass compositions.
- Additional ReaxFF parameter sets.
- New Stillinger-Weber parameters for AlGaN.
- New core-shell potential for InSnO (ITO).
- Minor performance improvements for CPU and GPU versions

Various GUI Updates

- Improved Graphics Support for Virtual Machines.
- The Data Tool, Builder, Workflow Builder, Viewer, and Database Tool windows are now embedded within the main interface, instead of opening as separate windows (watch video). Only the Editor and the Custom Scripter still open as windows.
- Added ability to extract and use custom quantities on Trajectory objects for coloring atoms in the Viewer.
- Updated Interface Builder.
- Enabled more precise drops in different available areas of a plot grid layout.





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