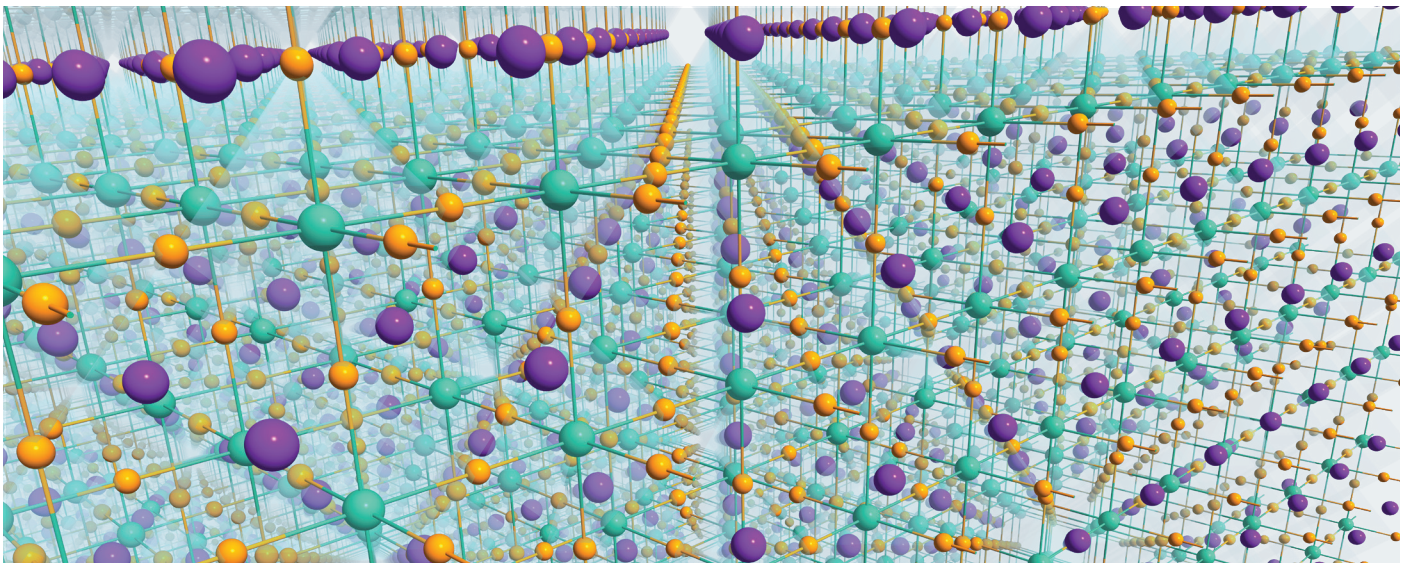
SYNOPSYS®

QuantumATK Release Features

Last amended: June 2021

QuantumATK S-2021.06

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 S-2021.06

Download

If you are a customer entitled to maintenance services, you can access QuantumATK S-2021.06 and download full release and installation notes directly from SolvNetPlus: https://solvnetplus.synopsys.com.

New Features in QuantumATK S-2021.06

Machine-Learned (ML) Force Fields | Moment Tensor Potentials (MTPs)

- 100-1000x faster generation of realistic structures of complex multi-element crystalline, amorphous materials & interfaces, defect and dopant migration barriers, thermal transport, crystallization vs. Density Functional Theory (DFT).
- Systematically improvable MTPs
  - Trained on a dataset of ab-initio calculations.
  - One of the most accurate and efficient ML potentials on the market. Nearly the same accuracy as ab-initio.
  - For cases where no conventional potentials exist or need better accuracy.
- Active learning MTP simulations to automatically add DFT training data during molecular dynamics (MD) simulations.
  - Obtain realistic amorphous material and liquid structures, in particular, at high temperatures.
- Employ provided MTP potentials for Si or develop potentials for new materials and problems using automated training and simulation workflows.
- Use MTPs with MD, nudged elastic band and accelerated MD methods, such as force-bias Monte Carlo, now also with pressure control, to sample rare events and unlock slow mechanisms.

Complex Semiconductor Materials, Interfaces & Gate Stacks

- Use ML MTPs for obtaining realistic crystalline, amorphous materials, interface, gate stack structures, simulating dopant diffusion, thermal transport, and crystallization.
  - Examples include amorphous HfO2 and GST phase-change materials, HKMG stacks, etc.
- Fast and highly accurate electronic properties of materials, interfaces, and gate stack (e.g. HKMGs) structures comprised of multiple layers with different band gaps using the dielectric dependent hybrid HSE06 (HSE06-DDH) method.
  - HSE06-DDH method is based on using improved material-specific fractions of exact exchange, automatically calculated from density for each material (in an interface).
  - Available with LCAO basis sets for efficient large-scale simulations with modest hardware.

- Geometry optimization with stress and spin-polarization is now available with HSE06-LCAO.
  - Accurate large-scale simulations of electronic properties orders of magnitude faster compared to HSE06-PlaneWave.
- New inverse participation ratio (IPR) analysis object to evaluate localized states
  - Part of the insightful electronic and vibrational analysis of systems with defects, amorphous materials, surfaces and interfaces, e.g., in HKMG and 3D-NAND memory stacks.
- Plot band edges in projected DOS, local DOS and projected local density of states analyzers.
- Defect and dopant simulation improvements
  - Easier set-up of individual defect migration paths.
  - Apply constraints and point defect symmetry to reduce the computational cost of defect diffusion simulations, e.g. at interfaces in HKMG stacks.

1D & 2D-Material Based FETs

- More accurate band diagrams and device I-V characteristics with the new HSE06-NEGF methodology compared to PBE-NEGF.
- More accurate on-state calculations using Neumann boundary conditions in the transport direction compared to Dirichlet at the Semi-Empirical level.
- Up to 80% faster simulations of gated devices with vacuum regions using the new Poisson solver using a non-uniform grid compared to the parallel conjugate gradient (PCG) solver.

Novel STT-MRAM Memory Design

- Obtain realistic interface structures and energetics of magnetic tunnel junctions in MRAM with ML MTPs.
- New magnetic properties such as Heisenberg exchange coupling, exchange stiffness, and Curie temperature.
- 10-100x faster Heisenberg exchange calculations, now also with non-collinear spin and spin-orbit.
- 60x times faster and 70 % less memory demanding magnetic anisotropy energy projection simulations.

Battery Materials Modeling & Design

Building

- Improved plugin for adsorbing molecules onto a surface and a new nanoparticle builder for creating a nanoparticle electrode.
- Improved move, measurement and atom wrapping tools.

ForceField Simulations

- New bonded OPLS potential for common electrolytes and OPLS-Min potential for use with custom charges and simpler type assignments.
- Convenient access to bonded potentials in the GUI and possibility to edit all terms, including torsion potentials.
- Large-scale solid-electrolyte-interphase (SEI) simulations using 3x faster ReaxFF Force Field MD or combined bonded and conventional potentials in the GUI.
- Easy set-up and simulations with partial charges to model electrostatic interactions using the GUI.
- Vibrational spectra from MD to understand molecular interactions and solvation in liquid phase.
- Surface process modeling and Thermochemistry analysis tools for modeling reactions on electrode surfaces.

Density Functional Theory Simulations

- More accurate electronic structure, binding energies, and diffusion barriers with the hybrid DFT functionals, such as HSE06 and the newly added PBE0, B3LYP, B3LYP5.
- Use LCAO basis sets for 100x speed-up compared to Plane Wave basis sets enabling highly efficient large-scale simulations with modest hardware.
- More accurate modeling of binding energy and adsorption sites with counterpoise corrections to DFT-NEGF.

Polymer Modeling

- Access bonded potentials (OPLS-AA, OPLS-Min, Dreiding, UFF) and edit them in the GUI for more convenient set-up of polymer simulations.
- Combine bonded and conventional potentials in the GUI for more accurate simulations of polymer-inorganic and polymer-nanoparticle interfaces.
- Graphically build and simulate polymer systems with ionically charged molecules using the QEq method, particularly relevant for photoresist polymers.
- GUI support for united atoms in the polymer building workflow to speed up polymer simulations by folding hydrogen atoms into their attached carbon atom.

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