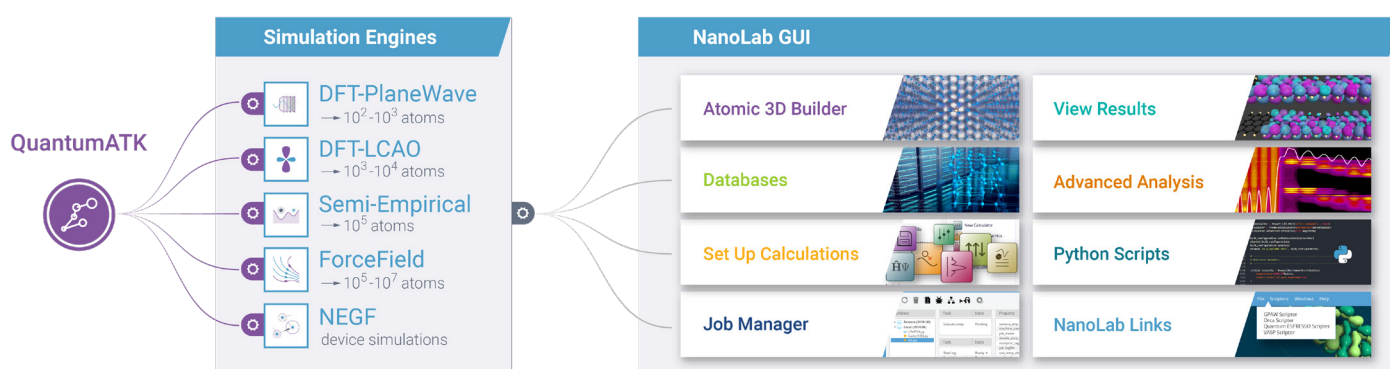


QuantumATK Platform for Universities & Government Labs

QuantumATK is a complete and fully integrated software suite for atomic-scale modeling for academic research, professionally engineered using state-of-the-art scientific and software-engineering methods. It combines the power of a Python scripting engine with the ease-of-use provided by an intuitive NanoLab graphical user interface (GUI). All simulation engines share a common infrastructure for analysis, ion dynamics, and parallel performance techniques.



Core Features of QuantumATK

NEGF Method of Nanoscale Device and Transport Simulations

Non-Equilibrium Green's function (NEGF) module works with DFT-LCAO, Semiempirical and ForceField Modules (see next page)

- ▶ **Types of Systems:** Nanoelectronic Devices & Interfaces (2-Probe), Surfaces (1-Probe)
- ▶ **Include:**
 - An effective doping scheme to simulate doped semiconductors
 - Metallic gate electrodes and dielectric screening regions
 - Surface, defect, interface, and grain boundary scattering effects
 - Electron-phonon coupling (EPC) effects (with BTE, MD-Landauer and STD-Landauer methods)
 - External electric fields
 - Relaxation of device geometries
 - Multilevel parallelism up to 1000s of cores
 - Options to balance performance vs. memory usage
- ▶ **Calculate:**
 - Electrical characteristics, such as I-V curves, on/off ratio, subthreshold slope, drain-source saturation voltage, drain-induced barrier lowering, transconductance
 - Transmission spectrum, eigenvalues, eigenchannels, device density of states (DOS), etc.
 - Schottky barriers and interface resistance (e.g. for metal-semiconductor contacts)
 - Thermal conductance/conductivity of materials, nanostructures, interfaces, etc.
 - Phonon-limited mobility and resistivity of materials
 - Tunnel magnetoresistance ratio, spin-polarized tunneling current, and bias-dependent spin-transfer torque for material stacks that comprise the magnetic tunnel junctions
 - Photocurrent and open circuit voltage for solar-cell devices and LEDs
 - Band-alignment, Schottky barriers, and work functions for thin film/surface heterostructures
 - Electronic surface states in external electric fields
 - Insight into catalytic activity of transition metal and transition metal oxide surfaces

Core Features of QuantumATK

- **DFT-LCAO:** Simulation engine for density functional theory (DFT) using pseudo-potentials and linear combinations of atomic orbitals (LCAO) basis sets.
- **DFT-PlaneWave:** Simulation engine for DFT using pseudo-potentials and plane-wave basis sets.
- **SemiEmpirical:** Semi-empirical simulation engine for using DFTB, extended Hückel, Slater-Koster, and other tight-binding models.
- **ForceField:** Simulation engine for atomic-scale simulations (e.g. molecular dynamics) using classical potentials.

DFT-PlaneWave

↑ 10^2 - 10^3 Atoms

DFT-LCAO

↑ 10^3 - 10^4 Atoms

SemiEmpirical

↑ 10^5 Atoms

ForceField

↑ 10^5 - 10^7 Atoms

► **Types of Systems:** Molecules, crystals, polycrystals, nanostructures, nanoparticles, alloys

•

•

•

•

► Works with NEGF method for simulations of nanoelectronic devices, interfaces, surfaces, solar-cells

•

•

•

► **Use:** More than 300 LDA/GGA/MetaGGA DFT functionals

•

•

► Hybrid functionals using the ACE approximation

•

► Van der Waals models: DFT-D2 and DFT-D3

•

•

► Hubbard U term for LDA and GGA

•

► Methods for accurate band gap calculations of semiconductors and insulators (MetaGGA, DFT-1/2, Pseudopotential Projector shift methods)

•

•

► Norm-conserving Troullier-Martins PPs (FHI, SG15/PseudoDojo)

•

•

► Predefined numerical atomic orbital basis sets for different accuracy levels

•

► Plane wave basis sets with automatic default cut-offs

•

► Spin settings: unpolarized, polarized, noncolinear, noncollinear spin-orbit

•

•

•

► Built-in Slater-Koster models for group IV and III-V semiconductors, extended Hückel model with over 300 basis sets and Tight-Binding models for strained systems

•

► More than 300 empirical classical potentials included, Python interface for adding your own or literature potential, support for custom combination of potentials

•

► **Perform:** Calculations of band structure, fat band structure, DOS, Fermi surface, cohesive energy, defect formation energies, and transition level, etc. calculations

•

•

•

► Geometry and unit cell optimization using LBFGS and FIRE methods

•

•

•

•

► Molecular dynamics (MD) (NPT, NVT, NVE, ..) simulations for studying mechanical (e.g. creep simulation), thermal properties, and physical processes (e.g. thin film growth); part of the MD-Landauer simulations to include electron-phonon coupling (EPC) effects

•

•

•

•

► Nudged elastic band (NEB) for reaction path optimization (e.g. to get insight into catalytic activity of transition metal and transition metal oxide surfaces)

•

•

•

•

► Adaptive kinetic Monte Carlo (AKMC) for long timescale kinetics (e.g. diffusion kinetics)

•

•

•

•

► Phonon modes (part of the STD-Landauer method to include EPC effects), phonon bandstructure, DOS, and thermal transport simulations

•

•

•

•

► **Benefit from:** Multilevel parallelism (threading + MPI) up to 1000s of cores. Parallelize over k-points/basis functions/NEB images/AKMC searches/bias points, etc.

•

•

•

•



Core Features of NanoLab GUI

NanoLab: Graphical User Interface (GUI) for all QuantumATK simulation engines: LCAO, PlaneWave, SemiEmpirical, ForceField and NEGF (transport).

Atomic 3D Builder

- ▶ Build your own molecules, crystals, nanostructures, etc. using advanced selection and move tools.
- ▶ Use 1st party plugins for setting up interfaces, nanowires, nanoparticles, polycrystals, alloys, cleave surfaces.
- ▶ Use Device tools for setting up device structures, including adding gate electrodes, dielectric screening regions, doping semiconductors.
- ▶ Set up and pre-optimize nudged elastic bands (NEB) reaction paths.
- ▶ Import ready-to-use structures from the internal NanoLab database and online databases such as Crystallography Online Database and Materials Project.
- ▶ Create your own internal databases using e.g. MongoDB or MySQL.
- ▶ Use Python console for having programmatic access to interact with the configurations in the Builder. Create pre-defined scripts to automate repeated tasks.

Visual Tool for Setting Up Calculations and Workflows

- ▶ Set up LCAO, PlaneWave, SemiEmpirical, ForceField, and NEGF calculations.
- ▶ Compute the electronic, optical, thermal, magnetic, mechanical, electron-phonon coupling, piezoelectric, thermoelectric, and other material properties of nanostructures, bulk materials, and surfaces.
- ▶ Use specialized interface to set up interdependent tasks for obtaining I-V characteristics, defect formation energies and transition levels.
- ▶ Set up molecular dynamics simulations using models such as NVT, NVE, NVT/NPT, etc.
- ▶ Optimize geometry (use the specialized interface for relaxation of devices and interfaces).
- ▶ Edit input files (python scripts) using the NanoLab editor.

Job Manager

- ▶ Submit and run jobs from the GUI in serial, using threading and in parallel using MPI.
- ▶ Submit jobs from the GUI to local or remote machines (Torque/PBS, LSF, SLURM).

3D Data Viewer/Movie Tool

- ▶ View optimized geometry, calculated Bloch states, fermi surface, electron (difference) density and other properties.
- ▶ Use interactive 3D measurement tool for distances and angles and use plugins to compare two configurations.
- ▶ Edit graphical properties, such as atom colour, background, light properties, etc.
- ▶ Visualize very large data sets (1M+ atoms and bonds).
- ▶ Export images and movies to most common graphical formats.
- ▶ Visualize the dynamics of MD trajectories, phonon vibrations, NEB paths, etc.

2D Plotting

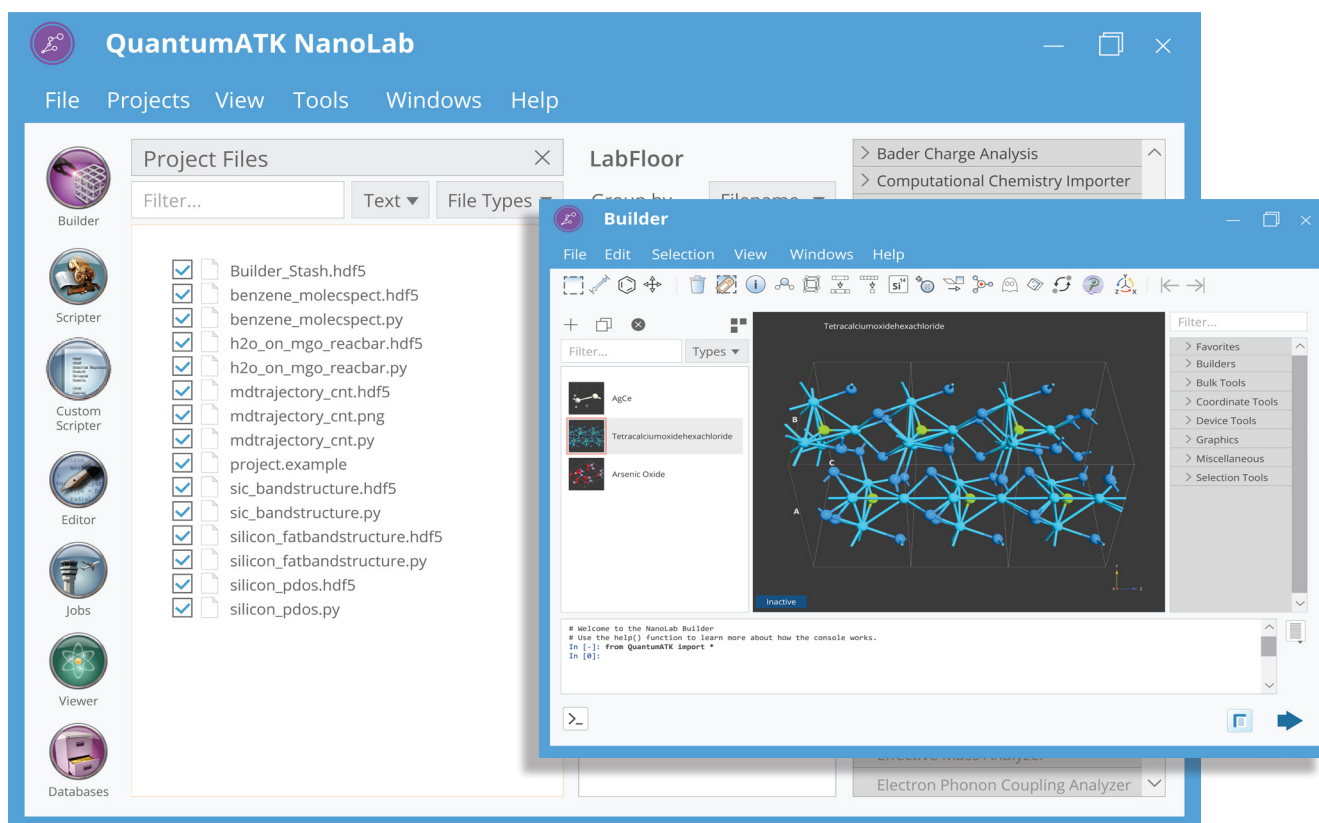
- ▶ Plot bandstructures, density of states (DOS), I-V curves, defect formation energies, optical spectrum, etc.
- ▶ Save and reuse customized plots.
- ▶ Combine plots, e.g. band structure and DOS.
- ▶ Add annotations like arrows and labels to plots.
- ▶ Modify titles, axis, grid lines, etc.

Project Management

- ▶ Organize data files into projects.
- ▶ Easily transfer projects between computers, or share with other users.
- ▶ Overview all data in a project, or focus on particular subsets, then combine data sets from different files for advanced analysis.

Plugin API

- ▶ Write addons and plugins in Python, using a simple API to add new functionality to NanoLab.
- ▶ Add support for additional external codes.
- ▶ Add new features to the NanoLab Builder (anything from simple operations to fully interactive widgets).
- ▶ Import/export of structures in external file formats.
- ▶ Add new data analysis capabilities and plot types.
- ▶ Use Add-on manager for installing plugins from server.
- ▶ Most functionality in NanoLab is plugin (addon) based.



Core Features of NanoLab Links

NanoLab Links: Module enabling NanoLab to interface other codes.

Interface to VASP

- ▶ Generate input files using interactive scripiter, supporting most VASP functionality.
- ▶ Add custom lines to and preview the INCAR file.
- ▶ Read data files for plotting and data analysis (OUTCAR, CONTCAR, CHGCAR, DOSCAR, EIGENVAL, CHG, PARCHG, ELFCAR, XDATCAR).
- ▶ Plot band structures, FatBandstructure (for analysis of the spd- and site projected character of the bandstructure), DOS, etc.
- ▶ Generate initial NEB paths using the IDPP method.
- ▶ Set up constraints.
- ▶ Visualize NEB paths and barriers.

Interface to QuantumESPRESSO

- ▶ Generate input files using interactive scripiter.
- ▶ Read and plot charge densities, DOS, band structures.
- ▶ Import trajectories generated by QuantumEspresso.

Interface to GPAW

- ▶ Generate input files using interactive scripiter.
- ▶ Read and plot charge densities.

Interface to Orca

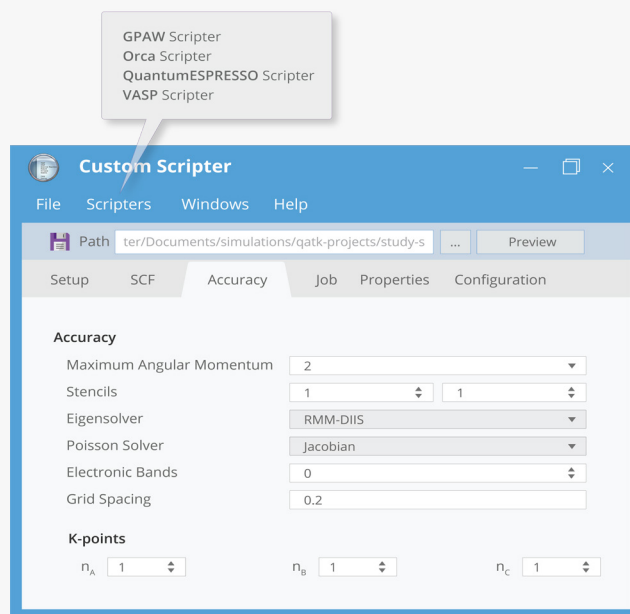
- ▶ Generate input files using interactive scripiter.
- ▶ Read and plot charge densities.

Interface to LAMMPS

- ▶ Create and export advanced structures.
- ▶ Import trajectories to make movies, calculate local structure, plot RDF, etc.

CCLib

- ▶ Import files from various quantum chemistry codes.



Synopsys
QuantumATK Team
Fruebjergvej 3
DK-2100 Copenhagen
DENMARK

www.synopsys.com/silicon/quantumatk.html
quantumatk@synopsys.com
+45 333 32 300

SYNOPSYS®

©2018 Synopsys, Inc. All rights reserved. Synopsys is a trademark of Synopsys, Inc. in the United States and other countries. A list of Synopsys trademarks is available at <https://www.synopsys.com/copyright.html>. All other names mentioned herein are trademarks of their respective owners.