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

[www.synopsys.com/silicon/quantumatk.html](http://www.synopsys.com/silicon/quantumatk.html)
### 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.

#### Types of Systems:
- Molecules, crystals, polycrystals, nanostructures, nanoparticles, alloys

#### 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, noncollinear, 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 scripter, 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 scripter.
- Read and plot charge densities, DOS, band structures.
- Import trajectories generated by QuantumEspresso.

### Interface to GPAW
- Generate input files using interactive scripter.
- Read and plot charge densities.

### Interface to Orca
- Generate input files using interactive scripter.
- 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.