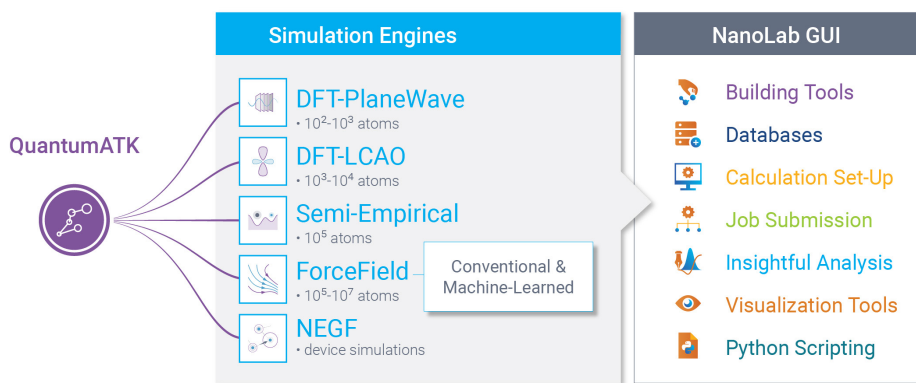# SYNOPSYS®

QuantumATK Platform for Materials Development

QuantumATK is a complete and fully integrated software suite for atomic-scale modeling of novel and complex materials, 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.

Simulation Engines	NanoLab GUI
QuantumATK	
DFT-PlaneWave · 10^2-10^3 atoms	Building Tools
DFT-LCAO · 10^3-10^4 atoms	Databases
Semi-Empirical · 10^5 atoms	Calculation Set-Up
ForceField · 10^5-10^7 atoms — Conventional & Machine-Learned	Job Submission
NEGF · device simulations	Insightful Analysis
	Visualization Tools
	Python Scripting

Core Features of QuantumATK

NEGF Method for 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, beyond slab approximation)

▶ **Include:**
- Surface, defect, interface, grain boundary scattering, and charge transfer effects
- External electric fields
- An effective doping scheme to simulate doped semiconductors
- Metallic gate electrodes, dielectric screening regions and implicit solvent models
- Electron-phonon coupling (EPC) effects: LOE and XLOE approximations for molecular contacts or nanostructures and one-shot SCBA approximation for bulk-like devices
- Relaxation of device geometries using BRR and NEGF methods w/wo constraints
- Multilevel parallelism up to 1000s of cores
- Options to balance performance vs. memory usage

▶ **Calculate:**
- 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
- Thermal conductance/conductivity of materials, nanostructures, interfaces, etc.
- 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.
- Phonon-limited mobility and resistivity of materials
- Tunnel magnetoresistance ratio, spin-polarized tunneling current, and bias-dependent spin-transfer torque
- Photocurrent and open circuit voltage for solar-cell devices and LEDs

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 (MD)) using classical potentials: Conventional and Machine-Learned.

	DFT-PlaneWave $\to 10^2$-10^3 Atoms	DFT-LCAO $\to 10^3$-10^4 Atoms	SemiEmpirical $\to 10^5$ Atoms	ForceField $\to 10^5$-10^7 Atoms
▶ **Types of Systems:** Molecules, (poly)crystals, amorphous, polymers, alloys, nanostructures, interfaces	●	●	●	●
▶ Works with NEGF method for simulations of nanoelectronic devices, interfaces, surfaces, solar-cells		●	●	●
▶ **Use:** More than 300 LDA/GGA/MetaGGA DFT functionals	●	●		
▶ Hybrid functionals (HSE06-(DDH), B3LYP, B3LYP5, PBE0)	●	●		
▶ 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	●	●		
▶ Norm-conserving Troullier-Martins PPs (FHI, SG15/PseudoDojo)	●	●		
▶ Projector-augmented wave (PAW) PP method	●			
▶ 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				●
▶ Machine-Learned Force Fields (ML FFs) for accurate dynamical simulations of amorphous materials, interfaces, phase transitions, thermal properties, diffusion, surface processes				●
▶ Pre-trained ML FF library and automated training workflows to generate new ML FFs				
▶ Gates, dielectric regios or implicit solvent models in devices or periodic structures		●	●	
▶ **Perform:** Calculations of band structure, fat band structure, (P)DOS, optical, magnetic properties, etc.	●	●	●	
▶ Spintronic properties, e.g. magnetic anisotropy energy, Heisenberg exchange, Gilbert damping		●		
▶ Boltzmann transport calculations of conductivity/mobility tensor, Hall coefficient and Hall conductivity tensor, Seebeck coefficient, and ZT including electron-phonon coupling (EPC)		●	●	
▶ 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, deposition, etching, sputtering). Part of the MD-Landauer simulations to include EPC effects	●	●	●	●
▶ Time-stamped force-bias Monte Carlo simulations as an alternative to MD for long time-scale equilibration, deposition, amorphization, diffusion, sampling of rare events	●	●	●	●
▶ Nudged elastic band (NEB) for reaction path optimization (e.g. to get insight into catalytic activity of transition metal and transition metal oxide surfaces, defect migration paths and energies)	●	●	●	●
▶ Adaptive kinetic Monte Carlo (AKMC) for long timescale kinetics (e.g. diffusion kinetics)		●	●	●
▶ Phonon modes (to include EPC effects), phonon bandstructure, DOS, and thermal transport	●	●	●	●
▶ **Benefit from:** Multilevel parallelism (threading + MPI) up to 1000s of cores. Parallelize over k-points/basis functions/NEB images/AKMC searches/bias points, etc.	●	●	●	●

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, multilayer stacks, grain boundaries, nanowires, nanoparticles, polycrystals, alloys, amorphous structures, cleave surfaces, adsorb molecules to a surface
- ► 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 DFT-LCAO, DFT-PlaneWave, SemiEmpirical, ForceField, and NEGF for device and transport simulations
- ► 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, magnetic anisotropy energy, 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 or write your own custom Python scripts
- ► Save your calculator settings/workflows as templates, reuse them in future calculations or share with colleagues
- ► Set up and submit large number of simulations at once for high-throughput material screening

Job Manager

- ► Submit and run jobs from the GUI in serial, using threading and in parallel using MPI, or OpenMP and MPI together
- ► Submit jobs from the GUI to local or remote machines (Torque/PBS, PBSPro, LSF, SGE, 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.
- ► Perform advanced editing of plots, such as changing color, line width, etc. of multiple items (several bands for instance) at once, changing title axes, legend, etc., editing grid layout, and adding annotations like arrows and labels
- ► Save customized plots for further analysis and reuse plot setups with new data
- ► Link and combine plots, e.g. band structure and DOS, for more insightful analysis
- ► Plot quantities along with the animation using a movie tool
- ► Fit data to linear and other models, apply smooth rolling or macroscopic averaging and measure directly in graphs
- ► Transform lines and adjust plot data range for analysis
- ► Manipulate plots in scripts and build your own custom plots

Report Generation

► Extract selected data from multiple calculations and perform analysis by expecting data in a table, grouping results, and visualizing extracted data (can also be saved in hdf5, csv or excel formats)
► Create and reuse research protocols, i.e., collection of predefined measurements with visualization

Project Management

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

Plugin API

► Write addons and plugins in Python, using a simple API to add new functionality to NanoLab
► Add new features to the NanoLab Builder (anything from simple operations to fully interactive widgets)
► Automate analysis and plotting, add new data analysis capabilities and plot types
► Use Add-on manager for installing plugins written by Synopsys QuantumATK team or users

GUI Interface to External Simulation Engines

► Generate input files and plot some of the data obtained with VASP, QuantumESPRESSO, GPAW, Orca, and LAMMPS
► Import/export structures in external file formats