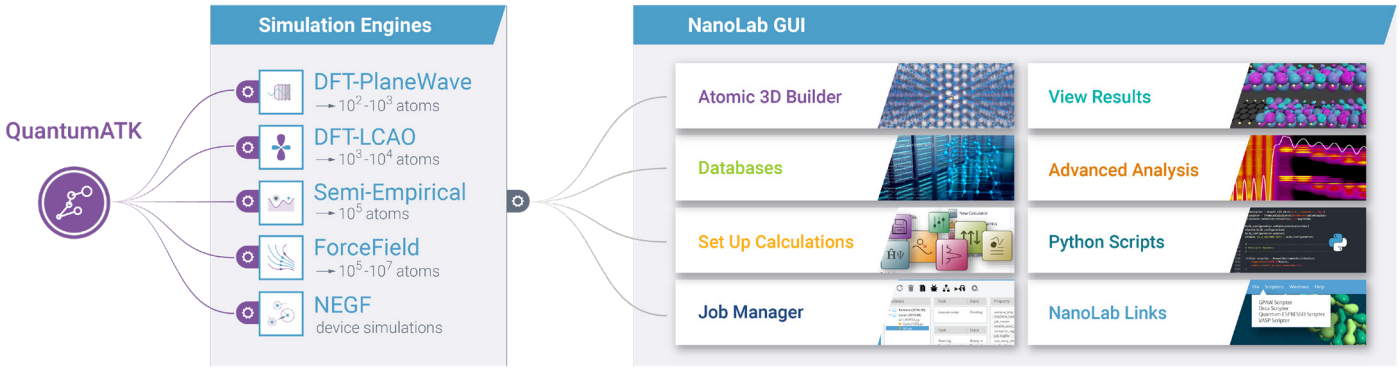
SYNOPSYS®

QuantumATK Simulation Engines for Advanced Semiconductor Development

QuantumATK is a complete and fully integrated software suite for atomic-scale modeling of semiconductors, 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. This datasheet describes QuantumATK simulation engines. You can download another datasheet on the NanoLab GUI.



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)
  - 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, interfaces in interconnect stacks)
  - Phonon-limited mobility and resistivity of materials (e.g. for interconnects and transistor channels applications)
  - Tunnel magnetoresistance ratio, spin-polarized tunneling current, and bias-dependent spin-transfer torque for material stacks that comprise the magnetic tunnel junctions in the STT-RAM bit cells
  - 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

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 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.	•	•	•	
▶ Geometry and unit cell optimization using LBFGS and FIRE methods	•	•	•	•
▶ Molecular dynamics (MD) (NPT, NVT, NVE, ..) simulations for studying atom dynamics, phonon and thermal transport, and physical processes (e.g. collapse of fins and pillars); part of the MD-Landauer simulations to include electron-phonon coupling (EPC) effects	•	•	•	•
▶ Nudged elastic band (NEB) for reaction path optimization (e.g. to calculate defect formation energies and migration barriers in materials, interconnect stacks)	•	•	•	•
▶ 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.	•	•	•	•

Synopsys
QuantumATK Team
Fruebjergvej 3
DK-2100 Copenhagen
DENMARK

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

SYNOPSYS®