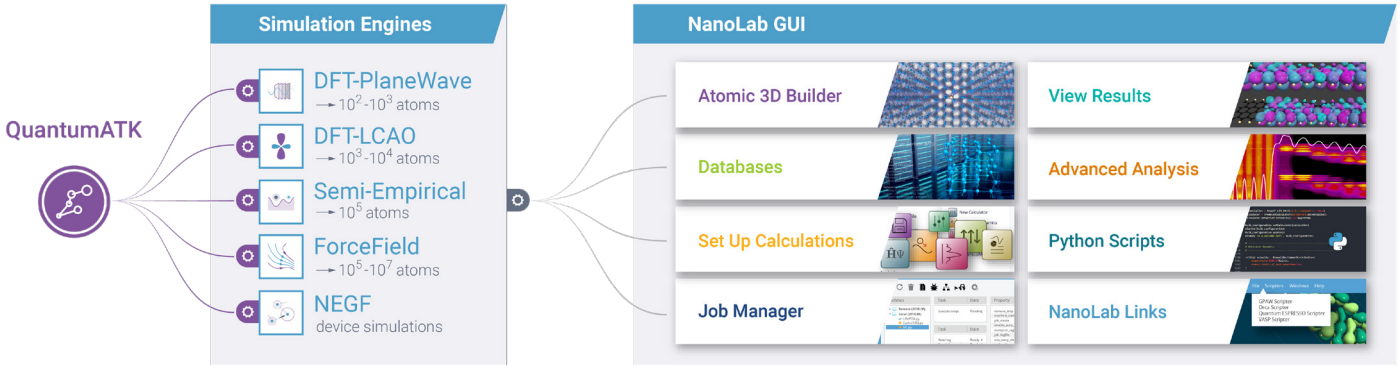
SYNOPSYS®

QuantumATK-M Simulation Engines for Materials Development

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



Core Features of QuantumATK-M

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 (MD-Landauer, STD-Landauer methods, and inelastic transmission methods)
  - 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 for material stacks that comprise the magnetic tunnel junctions
  - Photocurrent and open circuit voltage for solar-cell devices and LEDs

Core Features of QuantumATK-M

- **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.

	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, (poly)crystals, polymers, 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 (HSE06, 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 (Moment Tensor Potentials) where no conventional potential exists to describe complex materials accurately; automated training workflow to create & improve MTPs				•
▶ 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	•	•	•	
▶ 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 (NPT, NVT, NVE, ..) simulations for studying mechanical (e.g. creep simulation), thermal properties, and physical processes (e.g. deposition, etching, sputtering)	•	•	•	•
▶ 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)	•	•	•	•
▶ 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.	•	•	•	•

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