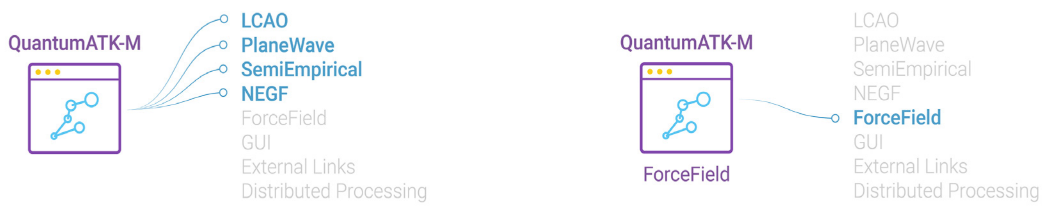
QuantumATK-M Products for Materials Development

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 two products: QuantumATK-M and QuantumATK-M ForceField. You can download another datasheet on the NanoLab GUI.



Core Features of the QuantumATK-M Product

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 (Surface Green's Functions method)
- **Include:**
  - Surface, defect, interface, and grain boundary scattering effects
  - Charge transfer effects
  - External electric fields
  - An effective doping scheme to simulate doped semiconductors
  - Metallic gate electrodes and dielectric screening regions
  - Electron-phonon coupling (EPC) effects (with BTE, MD-Landauer, and STD-Landauer methods)
  - Relaxation of device geometries
- **Obtain:**
  - Insight into catalytic activity of transition metal and transition metal oxide surfaces
  - Band-alignment, Schottky barriers, and work functions for thin film/surface heterostructures
  - Electronic surface states in external electric fields
  - 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
  - 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 OCV (open circuit voltage) for solar-cell devices and LEDs
- **Analyse:** Transmission spectrum, eigenvalues, eigenchannels, device density of states (DOS), etc

Core Features of QuantumATK-M and QuantumATK-M ForceField Products

- **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
QuantumATK-M Product	●	●	●	
QuantumATK-M ForceField Product				●
▶ **Types of Systems:** Molecules, (poly)crystals, polymers, nanostructures, 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, 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 potentials, support for custom combination of potentials				●
▶ **Perform:** Calculation of band structure, fat band structure, DOS, Fermi surface, cohesive energy, defect formation energies, and transition levels, etc.	●	●	●	
▶ 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 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	●	●	●	●

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