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
  - 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.

#### Types of Systems:
- Molecules, (poly)crystals, polymers, nanostructures, nanoparticles, alloys
- Works with NEGF method for simulations of nano electronic 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
- 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
- Gates, dielectric regions or implicit solvent models in devices or periodic structures

#### Perform:
- Calculations of band structure, fat band structure, (P)DOS, optical properties, and many more
- 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. thin film growth)
- 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)
- 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.