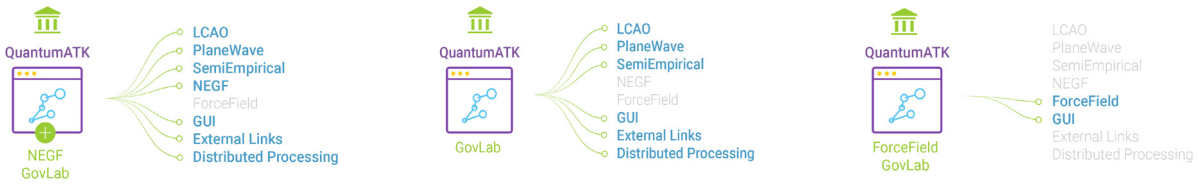
SYNOPSYS®

QuantumATK Products for Government Labs

QuantumATK is a complete and fully integrated software suite for atomic-scale modeling for academic research, 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 three products: QuantumATK + NEGF GovLab, QuantumATK GovLab, and QuantumATK ForceField GovLab.



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)
  - External electric fields
  - Relaxation of device geometries
- **Obtain:**
  - Electrical characteristics, such as I-V curves, on/off ratio, subthreshold slope, drain-source saturation voltage, drain-induced barrier lowering, transconductance
  - Schottky barriers and interface resistance (e.g. for metal-semiconductor contacts)
  - Thermal conductance/conductivity of materials, nanostructures, interfaces, 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 OCV (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
  - Insight into catalytic activity of transition metal and transition metal oxide surfaces
- **Analyse:** Transmission spectrum, eigenvalues, eigenchannels, device density of states (DOS), etc

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) 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 + NEGF GovLab and QuantumATK GovLab Product	●	●	●	
QuantumATK ForceField GovLab Product				●
▶ **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, 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:** Calculations 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	●	●	●	●

Core Features of QuantumATK NanoLab GUI

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, nanowires, nanoparticles, polycrystals, alloys, cleave surfaces.
- 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 LCAO, PlaneWave, SemiEmpirical, ForceField, and NEGF calculations.
- 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, 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.

Job Manager

- Submit and run jobs from the GUI in serial using threading and in parallel using MPI.
- Submit jobs from the GUI to local or remote machines (Torque/PBS, LSF, 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

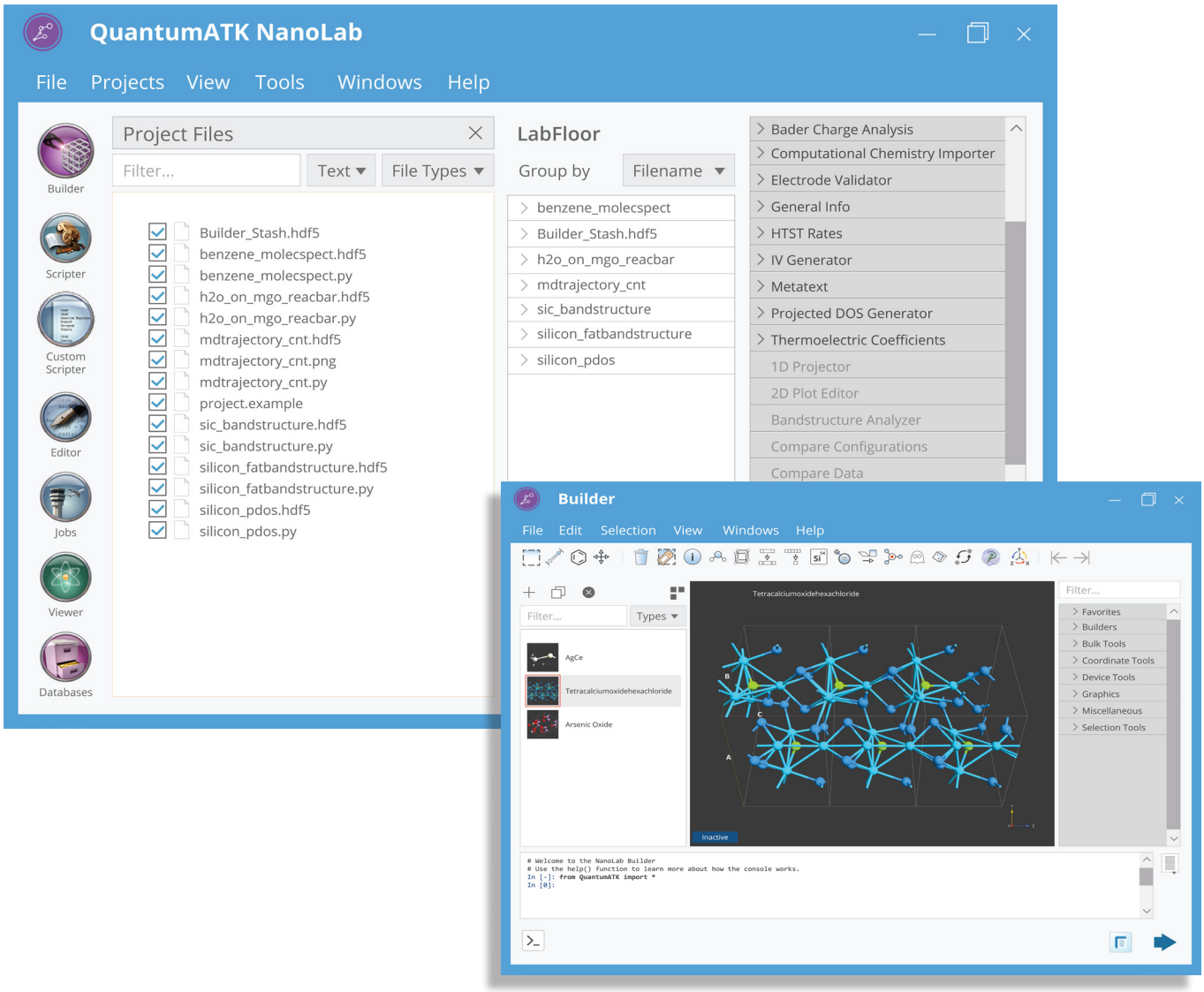
- Plot bandstructures, density of states (DOS), I-V curves, defect formation energies, optical spectrum, etc.
- Save and reuse customized plots.
- Combine plots, e.g. band structure and DOS.
- Add annotations like arrows and labels to plots.
- Modify titles, axis, grid lines, etc.

Project Management

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

Plugin API

- Write addons and plugins in Python, using a simple API to add new functionality to NanoLab.
- Add support for additional external codes.
- Add new features to the NanoLab Builder (anything from simple operations to fully interactive widgets).
- Import/export of structures in external file formats.
- Add new data analysis capabilities and plot types.
- Use Add-on manager for installing plugins from server.
- Most functionality in NanoLab is plugin (addon) based.



Core Features of NanoLab Links

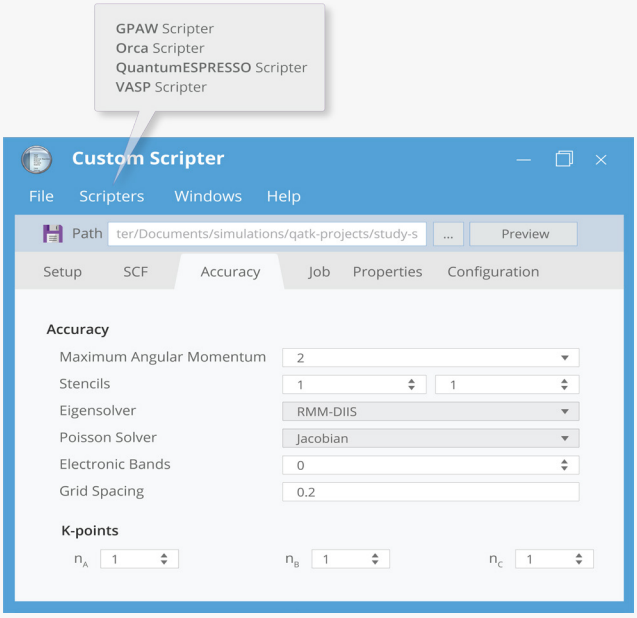
NanoLab Links: Module enabling NanoLab to interface other codes.

Interface to VASP

- Generate input files using interactive scripter, supporting most VASP functionality.
- Add custom lines to and preview the INCAR file.
- Read data files for plotting and data analysis (OUTCAR, CONTCAR, CHGCAR, DOSCAR, EIGENVAL, CHG, PARCHG, ELFCAR, XDATCAR).
- Plot band structures, FatBandstructure (for analysis of the spd- and site projected character of the bandstructure), DOS, etc.
- Generate initial NEB paths using the IDPP method.
- Set up constraints.
- Visualize NEB paths and barriers.

Interface to Quantum ESPRESSO

- Generate input files using interactive scripter.
- Read and plot charge densities, DOS, band structures.
- Import trajectories generated by Quantum ESPRESSO.



Interface to GPAW

- Generate input files using interactive scripter.
- Read and plot charge densities.

Interface to Orca

- Generate input files using interactive scripter.
- Read and plot charge densities.

Interface to LAMMPS

- Create and export advanced structures.
- Import trajectories to make movies, calculate local structure, plot RDF, etc.

CCLib

- Import files from various quantum chemistry codes.

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