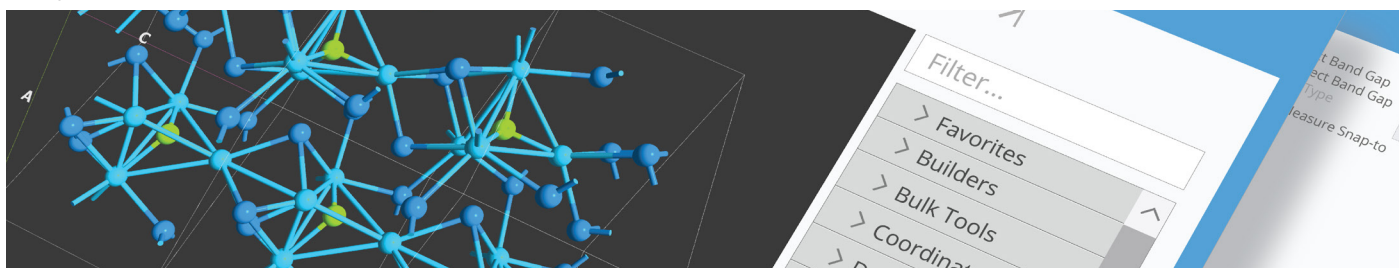


QuantumATK-M NanoLab GUI for Materials Development

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. All simulation engines share a common infrastructure for analysis, ion dynamics and parallel performance techniques.



Core Features of NanoLab GUI

NanoLab: Graphical User Interface (GUI) for all QuantumATK-M 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, grain boundaries, nanowires, nanoparticles, polycrystals, alloys, amorphous structures, 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, for ex., 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 DFT-LCAO, DFT-PlaneWave, SemiEmpirical, ForceField, and NEGF for device and transport simulations.
- ▶ 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, magnetic anisotropy energy, 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.
- ▶ Save your calculator settings and workflows as templates, reuse them in future calculations or ship them to your colleagues

Job Manager

- ▶ Submit and run jobs from the GUI in serial, using threading and in parallel using MPI, or OpenMP and MPI together.
- ▶ Submit jobs from the GUI to local or remote machines (Torque/PBS, PBSPro, LSF, SGE, 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.
- ▶ Perform advanced editing of plots, such as changing color, line, width, etc. of multiple items (several bands for instance) at once, changing title axes, legend, etc., editing grid layout, and adding annotations like arrows and labels.
- ▶ Save customized plots for further analysis and reuse plot setups with new data.
- ▶ Link and combine plots, e.g. band structure and DOS, for more insightful analysis.
- ▶ Plot quantities along with the animation using a movie tool.
- ▶ Fit data to linear and other models, apply smooth rolling or macroscopic averaging and measure directly in graphs.

Report Generation

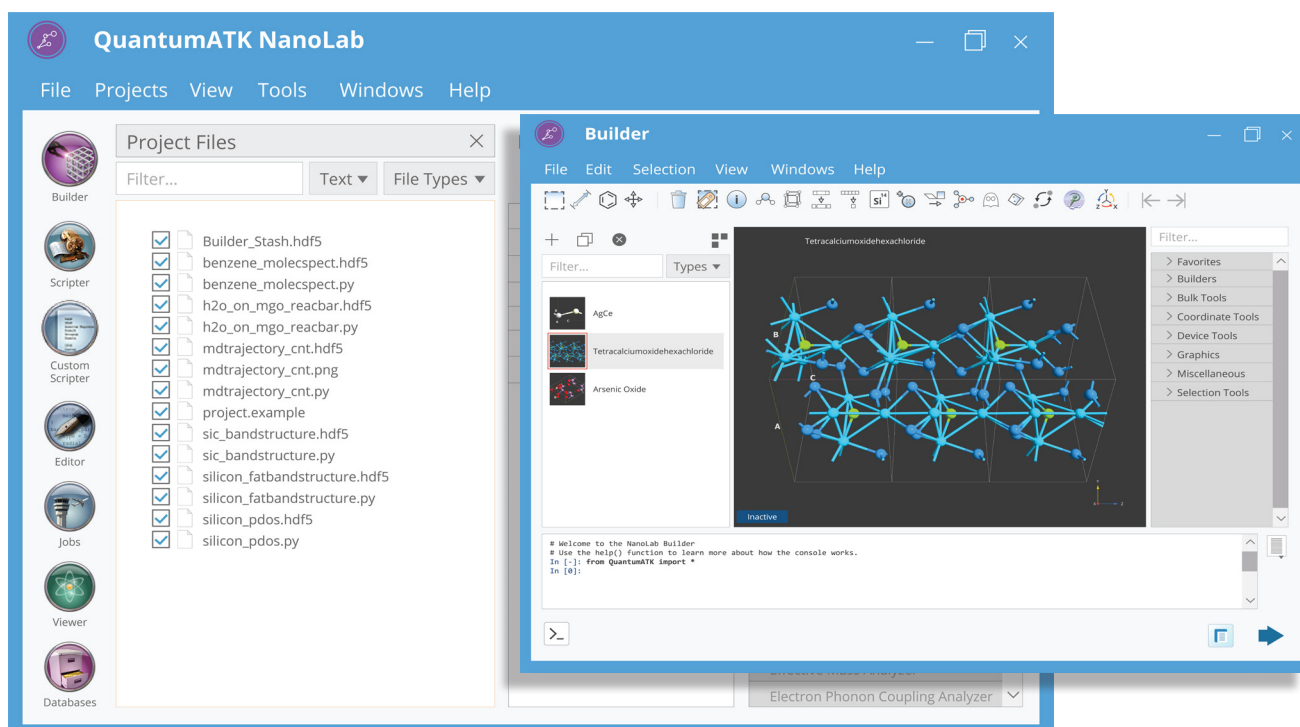
- ▶ Extract selected data from multiple calculations and perform analysis by exporting data in a table, grouping results, and visualizing extracted data.

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 written by Synopsys QuantumATK team or users.
- ▶ 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 scripeter, 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 QuantumESPRESSO

- ▶ Generate input files using interactive scripeter.
- ▶ Read and plot charge densities, DOS, band structures.
- ▶ Import trajectories generated by QuantumEspresso.

Interface to GPAW

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

Interface to Orca

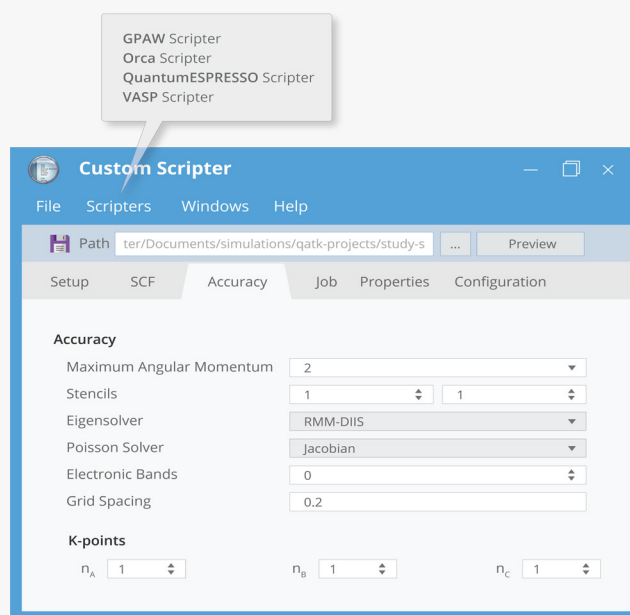
- ▶ Generate input files using interactive scripeter.
- ▶ Read and plot charge densities.

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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