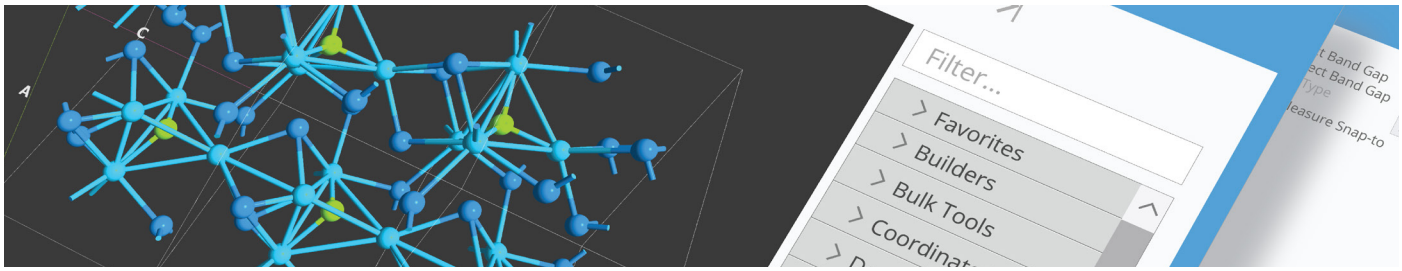
SYNOPSYS®

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, 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, 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 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

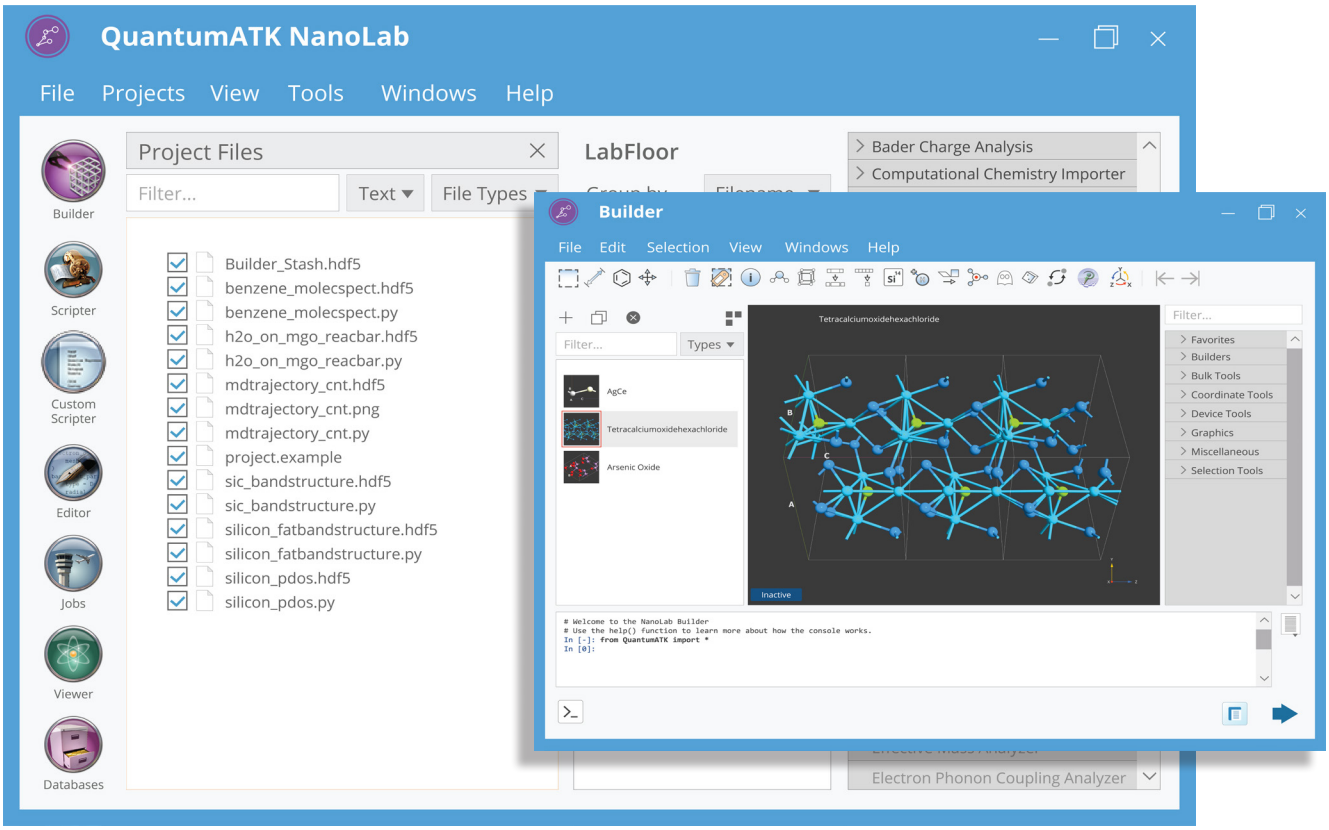
- Plot bandstructures, density of states (DOS), I-V curves, defect formation energies, optical spectrum, etc.
- Save and reuse customized plots.
- Combine plots, e.g. band structure and DOS.
- Add annotations like arrows and labels to plots.
- Modify titles, axis, grid lines, etc.

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

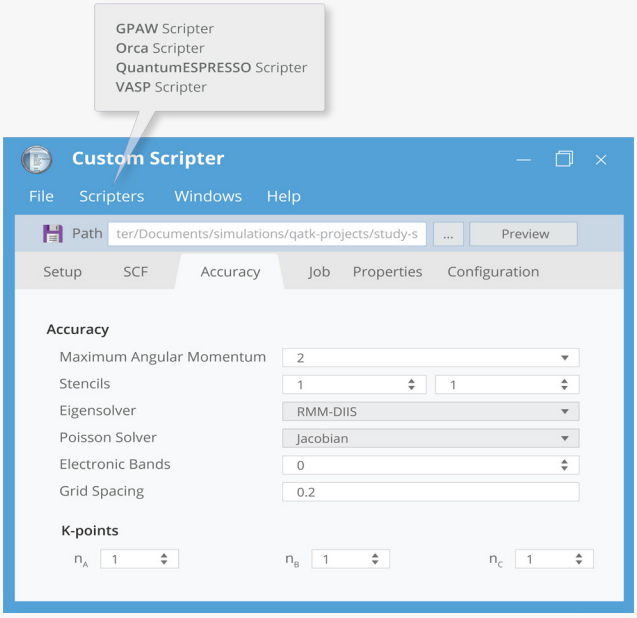
NanoLab Links: Module enabling NanoLab to interface other codes.

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 QuantumESPRESSO

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



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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