

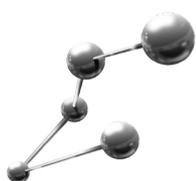
# ATK-VNL

## Release Features

### Version 2013.8

Last amended: June 2013

## ATK-VNL 2013.8



ATK-VNL is a leading industry-proven platform for atomic-scale modeling of materials, nanostructures, and nanoelectronic devices. It includes quantum mechanical methods such as density functional theory (DFT) with either LCAO or plane-wave basis sets and semi-empirical models, simulation engine for atomic-scale simulations using classical potentials, module for nanoscale device and transport simulations using non-equilibrium Green's function (NEGF) methodology. ATK-VNL combines the power of a Python scripting engine with the ease-of-use provided by an intuitive graphical user interface, Virtual NanoLab. All simulation engines share a common infrastructure for analysis, ion dynamics and parallel performance techniques.

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### New Interface | Introducing Projects and the LabFloor

- ▶ Group your files into projects
- ▶ Easier and more transparent access to objects in NetCDF files
- ▶ Complete overview of all files and data within a project on the LabFloor
- ▶ Combine data sets from different files for analysis
- ▶ The Builder "stash" is now persistent across sessions - and separate for different projects
- ▶ But - if you like the old interface, you can also make ATK 13.8 look like 12.8 and still benefit from all the new features.
- ▶ This is also handy for quickly navigating around your directory structure to locate a file.
- ▶ Transmission Analyzer - investigate specific transmission spectra in more detail. Calculate transmission eigenvalues and eigenstates interactively.
- ▶ Enhanced band structure analyzer - e.g. measure band gaps.
- ▶ Plotting tool for 3D grids projected to 1D
- ▶ Defined by plugins - expect more, and write your own!

### IV Curves

- ▶ Easily set up, compute, and and plot I-V curves
- ▶ Investigate the transmission spectra behind the calculation.
- ▶ The dynamical view in the I-V plot plugin allows you to symmetrize the curve.
- ▶ Click a voltage point to highlight the transmission spectrum.

### Phonon Calculations

- ▶ Phonon band structure and density of states for bulk materials, nanowires, nanotubes, graphene, etc.
- ▶ Study thermal transport - compute the phonon transmission spectrum and calculate the Seebeck and other thermal coefficients
- ▶ Parallelized with near-linear scaling up to 3N nodes (N=the number of atoms)

### Noncollinear Spin

- ▶ Available for both electronic structure and transport calculations
- ▶ Specially developed novel methods for improved convergence, using a collinear initial state

### Crystal Builder

- ▶ Build crystals from scratch, using Wyckoff positions
- ▶ Strukturbericht templates
- ▶ Symmetry recognition (spglib) - plugin the Builder

### New 3D Viewer

- ▶ Improved performance for trajectory movies and large structures
- ▶ Control atom color, radius etc individually
- ▶ Set background color, control lighting in detail
- ▶ Set atom properties by properties, like radius by Mulliken population or color by effective potential or forces (requires plugins)
- ▶ Better support for old graphics drivers - performance may suffer, but at least VNL starts up properly.
- ▶ Easy export of images from the Builder and Viewer in various bitmap formats.
- ▶ There is also an update to the POVRay plugin for generating ray-traced images

## Doped Systems

- ▶ Doping can also be introduced in the central region (earlier it was only possible to do for the electrodes) via so-called compensation charges. This allows for simulations of a wide variety of semiconductor devices, like p-n junctions, p-i-n doped Si nanowires, etc, without the need to introduce explicit dopant atoms.
- ▶ Doping charge can now be set in Scriptor; the compensation.
- ▶ Improved convergence of doped device systems.

## Molecular Dynamics

- ▶ Large set of Tersoff potentials from Tremolo-X
- ▶ Pre/post step hooks for customized on-the-fly analysis or time-dependent modifications of the structure (to make a stress/strain curve, for instance)
- ▶ NVT, NPT, NVTBerendsen, NPTBerendsen, Velocity Verlet

## Plane Wave Method: ABINIT

- ▶ Shipped with ATK 13.8 - both for Linux and Windows, with support for MPI parallelization
- ▶ Fully integrated with the ATK Python scripting language for total energy, NEB, geometry optimization and band structure calculations
- ▶ Other customized ABINIT tasks can be scripted too

## Method Improvements

- ▶ ATK-SemiEmpirical
  - All models now available in fully nonself-consistent and selfconsistent form
  - Performance enhancements
- ▶ New shell-wise Hubbard +U model
- ▶ Counterpoise correction to compensate for the basis set superposition error (BSSE). Use this when optimizing molecules on surfaces etc to get high accuracy.
- ▶ Grimme's DFT-D2 semi-empirical model for van der Waals interactions, both forces and stress; parameters for most elements up to Xe
- ▶ Multigrid method
  - Added support for non-orthogonal cells
  - Performance improvements

## Smaller Changes, Improvements and Additions

- ▶ The keyword `grid_mesh_cutoff` for `NumericalAccuracyParameters` has been renamed to `density_mesh_cutoff` which is more correct conceptually. The old keyword is still accepted for backwards compatibility.
- ▶ It is now possible to save arbitrary numpy arrays in NC files. This is very handy when you have computed some results - possibly in a time-consuming post-processing step - and want to store them for later plotting etc.
- ▶ Several small improvements to the Interface Builder, like a small inaccuracy in the positions of plot points in the surface cell picker, shift in Z kept consistent when adding layers, and the default suggestion for the surface cell is now really the smallest cell.
- ▶ Device from Bulk - algorithmic improvements and new presentation of electrode Z-length choices.
- ▶ A few performance improvements related to MD simulations and other cases where a copy is needed of a configuration.
- ▶ Unit cells and coordinates are now slightly rounded to avoid 0 being represented as 1e-17 in generated scripts.
- ▶ No question anymore for permission to overwrite existing NC files - ATK doesn't actually overwrite existing NC files, it just appends to them (normally, at least - unless you use an object ID already present in the file).

- ▶ Memory Usage button in the Script Generator to provide an estimate of the required memory for a calculation. Can also be inserted in a script, since the estimate can take some time. See the dedicated tutorial for more details.
- ▶ Transmission spectrum is now always identically zero for energies where there are no propagating states. This means you can trust that a small but non-zero value is not just numerical noise but actually indicates finite but small transmission.
- ▶ Clearer which stash items you are about to delete.
- ▶ Possibility to make the stash panel in the Builder larger.
- ▶ The scipy package is now part of ATK.
- ▶ Clearer error messages in cases where licenses (trial or usual ones) have expired.

## Bugfix Update VNL-ATK 2013.8.1

### Serious Bugs Fixed (Which Could Give Incorrect Results in Calculations!)

- ▶ The wrong set of k-points for hexagonal (and other) lattices were generated by the symmetry recognition routines in ATK in some cases, which could result in incorrect results for the density of states. In 13.8.1 this is solved by not using symmetries at all - this makes the calculations take a bit longer of course. In 14.2 the correct symmetry points will be used.
- ▶ The Cleaver was unable to cleave for instance base-centered orthorhombic crystals correctly. Also, there were issues when you manually rotated the cell - even if you chose an "electrode" cell, C was not perpendicular to the AB plane always.
- ▶ The dynamical matrix calculation now employs the acoustic sum rule and symmetries to avoid negative frequencies.
- ▶ A degeneracy factor was missing for the entropy of phonon DOS.
- ▶ The function sortCoordinates (used e.g. in the "Coordinate list" plugin) would fail for systems with many atoms, leaving the atoms unsorted. This was especially a problem for large devices which rely on this sorting for the central region to reduce memory usage (and indeed construct the device using "Device from Bulk").
- ▶ A Bohr/Angstrom mixup in QuantumEspresso import caused incorrect structures if the input file was specified in Bohr.
- ▶ Errors with Tersoff potentials for III-V alloys (Tersoff\_GaAs\_2002, Tersoff\_GaAs\_2011 and Tersoff\_InGaAs\_2000) have been corrected (the errors are actually in the original references themselves).

### Additions & Improvements

- ▶ LDOS for ATK-SE has been implemented.
- ▶ Thermal transport coefficients can now be plotted as a function of the Fermi level (image to the right)
- ▶ ElectrodeValidator function - new way to find proper electrode sizes (will be presented in the new ATK device tutorial)
- ▶ Adding more information to the About box, to help diagnose OpenGL issues. Also possible to email the information directly to QuantumWise.
- ▶ ElectronDifferenceDensity now calculates all spin components.
- ▶ All files are unchecked by default in new projects, to avoid a large new project taking very long time to load.
- ▶ The dynamical matrix is no longer recalculated for devices each time - now it will be reused if it has already been calculated.
- ▶ The colorbar is now included in exported images.
- ▶ Export Abinit scripts to a directory without actually running them (this is not supported from the Script Generator though, you have to add a line in the script).
- ▶ Band structure plots etc now have window titles so you know which file they come from.
- ▶ The object ID is shown in the tooltips for items imported to the LabFloor from NC files.
- ▶ You can now delete files using the keyboard (Del button) in the file panel of the main VNL window.

- ▶ The Installation guide has been added to the Start Menu.
- ▶ Sorting of the projects in the "Open project" dialog has been disabled because sorting caused the wrong project to be opened when you selected it.
- ▶ LabFloor importers now give item titles to FHI and QuantumEspresso files.
- ▶ The scrollbars on the LabFloor work better now.

## Noticeable But Not Severe Bugs

- ▶ It was not possible to select multiple images in a NEB path in the Builder - and thus not possible to apply operations like Translate etc to many images at once.
- ▶ The Script Generator made incorrect scripts for GGA and MGGA with ABINIT.
- ▶ Spin-polarized device calculations using DFTB now works - the equivalent bulk was not polarized which caused a segfault when going into the device part.
- ▶ When exporting matplotlib data, the global normalization factor was not removed, so the data was not scaled properly.
- ▶ Running MemoryUsage for device using a DFTB calculator now works.
- ▶ Cut Planes in the Viewer would not display negative values.
- ▶ Running a quick optimization with the Brenner potential made it impossible to insert a spatial region.
- ▶ LDOS was not supported in the Projector1D plugin
- ▶ Crystal Builder: if the first inserted point is (x,y,z), editing coordinates didn't work.
- ▶ The NEB builder progress bar appeared behind the Builder and the "Create" button could easily be clicked multiple times inf you didn't notice it was already running.
- ▶ Cut Planes in the Viewer - the preset planes AC and BC were reversed.

## Smaller Stuff

- ▶ A smaller Bohr/Angstrom mixup for unit cells has been fixed.
- ▶ "Analysis from File" (and a few other file dialogs) did not always open up in the project directory.
- ▶ Crystal Builder: the default unique axis for Monoclinic should be B
- ▶ The discs at the end of bonds were not transparent.
- ▶ filename.nc was written twice when LabFloor items were grouped by calculator ID
- ▶ Classic mode started in the wrong directory sometimes.
- ▶ Copy atoms is no longer possible for NEB configurations in plugins like Translate etc (it doesn't make sense).

## Unfixed Known Issues

- ▶ Running Abinit in parallel requires special setup of the cluster, and even with that it sometimes doesn't work properly. We are investigating the issue but don't expect to have a fix until ATK 14.2.
- ▶ Sometimes you click the "Create" button in the I-V Curve generator but nothing happens. Solution: try again! It's because of a conflict with the file being locked for reading by the LabFloor, and the file is unavailable for writing a short period after that.
- ▶ Coloring of isosurfaces for Bloch states is wrong.
- ▶ Reloading plugins raises errors if any atoms are selected when the reload is requested. Workaround: unselect all atoms first.

## Bug Fixes (Compared to 12.8.2)

- ▶ Trajectories where the cell changes were not read correctly (nload).
- ▶ The method "lastImage()" for trajectories now works as intended.
- ▶ MoS2 and MoSe2 structures corrected in the Database (cf. Phys. Chem. Chem. Phys. 4, 4078 (2002)).
- ▶ Sealed a memory leak (self-energies) in device calculations.
- ▶ Forces for non-selfconsistent Slater-Koster models corrected.
- ▶ EMTCalculator ignored repeated images and therefore did not work correctly for bulk configurations.
- ▶ No matter which k-point sampling you set in C, the Script Generator always generated the script with 100 points, which is always a safe choice, so it's not a serious problem, but anyway fixed now.
- ▶ The maximum number of steps set for an optimization will now apply also to a stress optimization. Earlier the loop over stress would run forever if the criterion was not met.
- ▶ Better handling of zero (or very small) or very large values of the lattice parameters (could force the Builder to crash). Also improved error messages for illegal lattice parameters.
- ▶ Tags are now kept when systems are dragged and dropped onto each other in the Builder.
- ▶ The "Fit cell" plugin has been improved for some difficult cases.
- ▶ Passivate tool could cause VNL to segfault for some structures - fixed.
- ▶ Z-matrix tool now handles the selection order of atoms correctly when switching stash items.
- ▶ Spatial regions inside electrodes are now displayed correctly in the Builder and Viewer (and not shifted inside the central region as before).
- ▶ Better handling of rare cases where atoms are deleted in the electrodes causing the device to become invalid.
- ▶ Contour integral parameters now cloned correctly when upgrading a calculator.
- ▶ Ctrl and Shift not always observed when clicking the 3D view when the Builder is not active.
- ▶ Cube file export no longer prints the trailing line which could trip up some other programs that import Cube files.
- ▶ Improvements to the license configuration tool, to correct for mistakenly set server port.
- ▶ Effective Mass Analyzer prints unit for Cartesian k-points - was confusing that they appeared in 1/Bohr when most other output in ATK is in Angstrom.
- ▶ The NEB preoptimization also uses the max\_steps keyword set for the NEB calculation itself.
- ▶ Eigenstates, small bug related to using default quantum numbers.
- ▶ Again possible to add an extra image between other ones in a NEB path - worked in 12.2 but not in 12.8.
- ▶ Ti-beta actually generated a structure with a Tl (thallium) atom - typo...
- ▶ Nanowire plugin doesn't crash anymore when using a small radius
- ▶ ... plus a few really small and esoteric issues



### Synopsys QuantumATK Team

Fruebjergvej 3  
DK-2100 Copenhagen  
DENMARK  
Tel: +45 333 32 300  
Email: [quantumatk@synopsys.com](mailto:quantumatk@synopsys.com)