

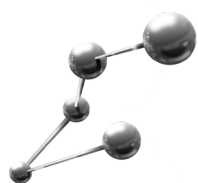
ATK-VNL

Release Features

Version 2017

Last amended: June 2017

ATK-VNL 2017



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.

▶ New Features in ATK-VNL 2017	2
• Electron-Phonon Calculations	2
• General Performance Improvements	2
• New Methods for Band Gaps	3
• New Storage File Format: HDF5	3
• Database Connectivity	3
• Wigner-Seitz Approximation for Large Supercells	4
• Ion Dynamics	4
• New Builder Features	4
• New Analysis Features	5
• Script Generator Updates (New Defaults)	5
• Job Manager Updates	5
• 3D Plotting	6
• 2D Plotting	6
• ATK-PlaneWave	6
• Platform Updates	6
• Miscellaneous	7
▶ Bugfix Update VNL-ATK 2017.2	7
▶ Bugfix Update VNL-ATK 2017.1	8

Electron-Phonon Calculations

- ▶ **Significantly lower memory requirement by storing all matrices as sparse**
 - For one calculation it was benchmarked to go from 800 GB to 1.3 GB!
- ▶ **New approximation for calculating mobility: constant relaxation time (similar to the Boltztrap code).**
 - The relaxation time can be provided, e.g. from experiments, but can also be computed from the dynamical matrix and averaged over energy/k-space
- ▶ **For devices which are just a repetition of the electrodes along the entire transport direction (like a long, simple nanowire, nanotube, or 2D slab), the inelastic current calculations can be run up to 100,000 times faster by only calculating the dynamical matrix and dH/dR for the electrode**
- ▶ **Gain 10-100x in performance by grouping (summing) all phonon modes in an energy range, as an approximation**

ATK 2017 introduces a novel so-called **Special Thermal Displacement (STD)** approximation to capture the effect of phonon scattering on the I-V curve. The "STD-Landauer" method is presented in more detail in [arXiv:1706.09290](https://arxiv.org/abs/1706.09290), but basically it reduces the complete electron-phonon coupling calculation to the evaluation of the dynamical matrix of the central region (also needed for LOE/XLOE) and a single device calculation for each bias (and temperature). The idea is to create a single distorted atomic configuration based on a canonical average over all phonon modes, in order to encapsulate all temperature effects.

The article demonstrates how this method can be used to very efficiently evaluate the phonon influence on the electronic current for a p-n Si junction device, as well as the mobility of Si bulk and nanowires as a function of temperature (see right).

General Performance Improvements

- ▶ **Number of "bands above Fermi level" is now set automatically**
 - Usually gives 2x in performance; it could be done manually before, but most users did not notice this option
- ▶ **New storage options for self-energies:**
 - NoStorage (drastically reduces memory usage for large devices, but requires recalculation in each step)
 - SaveInMemory (fast, but requires memory)
 - StoreOnDisk (fast, almost no memory requirement, uses disk space instead)
 - Reuse self-energies between calculations, when using the same electrodes for different central regions
- ▶ **SparseGreensFunction improved**
 - Use to reduce memory usage for large cross sections
 - Especially for finite bias, using multiple processes per contour point provides significant memory reduction per MPI process
- ▶ **No performance overhead anymore for the distributed Pulay mixer (now default)**
- ▶ **Detect automatically if electrodes are "identical" even if shifted a bit (can be turned off)**
- ▶ **Self-energy caching improvements**
- ▶ **Grid operations (10% memory cost for 20% performance gain in real-space integration)**

New Methods for Band Gaps

- ▶ **DFT+1/2**
 - Semi-empirical DFT approach to correct the self-interaction error in local and semi-local exchange-correlation functionals
 - Known from literature (Ferreira *et al.*, 2008 and 2011) and builds on Slater's half-occupation method
 - "More ab initio" than other methods like MGGA or GGA+U, since the parameters seem more transferable, i.e. you don't necessarily need to fit the parameters for each material individually. Testing shows that the same parameters can cover a class of materials, e.g. oxides with the same oxidation state, without any additional parameters needed for the metal ion, or III-V alloys with a universal anion parameter set.
 - Pre-defined parameters provided for oxygen (for simple oxides), Si, III-V and II-VI alloys
 - Not recommended for force/stress optimizations
- ▶ **Pseudopotential projector shifts (PPS)**
 - Novel method developed by QuantumWise which introduces adjustable parameters into the pseudopotential to improve properties like band gaps and lattice constants, similar in spirit to the empirical pseudopotential method but still based on DFT. The parameters are fitted for a reference system (like bulk Si) but appear to be transferable to e.g. alloys and nanowires.
 - Parameters are provided for Si and Ge, in the form of predefined pseudopotentials. We have successfully used these to describe the dependence of both the lattice constant and band gaps on the composition x of $\text{Si}_{1-x}\text{Ge}_x$ (see right).
 - Works for phonons too, if calibrated accurately.

New Storage File Format: HDF5

As of ATK 2017, the default storage format is now HDF5. As a user, you should not really notice any difference, except that the extension has changed. Technically, however, the HDF5 format offers possibilities for new features and performance.

- ▶ **Annotate your calculations, by adding "metatext" to HDF5 objects (calculators, band structures, any object)**
- ▶ **Remove data from HDF5 files**
- ▶ **Better parallel performance**
- ▶ **Significantly better performance for classical MD when using HDF5 files for trajectories**

Note: All old NC files are still compatible with VNL and ATK 2017 (for reading).

Database Connectivity

- ▶ **Access the [Materials Project](#) database from VNL**
 - Search for combinations of elements, crystal structure, and other parameters
 - View matches in a table view showing key properties, and visualize the structure
 - Import the crystal structures to VNL, as well as results such as band structure, DOS, etc, and visualize them directly in VNL
 - Improved functionality of the [Crystallography Open Database \(COD\)](#) interface
- ▶ **Improved functionality of the [Crystallography Open Database \(COD\)](#) interface**
- ▶ **By writing a custom plugin, create an interface to any MySQL or MongoDB database**
- ▶ **Create your own database of ATK calculations**

Wigner-Seitz Approximation for Large Supercells

Anyone who ever tried to calculate phonons in large supercells knows that this can be a prohibitively expensive exercise, due to the need to repeat the cell at least three times in each periodic direction. Thus even a “small” supercell with say 100 atoms turns into 600 calculations of a system containing 2700 atoms.

ATK 2017 solves this problem by introducing a novel and innovative approximation based on a Wigner-Seitz partition of the forces, such that atoms that are far from each other in the original supercell (on opposite edges, for instance) do not feel the forces of the repeated-image atoms under periodic boundary conditions.

Using this approximation it is possible to obtain both accurate phonon band structures and vibrational eigenmodes without repeating the cell (“poor man’s frozen phonon calculation”). The approximation becomes exact in the limit of large supercells, but has good accuracy already at 3x3x3, esp. for the acoustic phonon DOS.

The accuracy of the method is demonstrated in the figures on the right, which show the phonon DOS and band structure of a 63-atoms Si vacancy system.

Timings:

- ▶ Reference calculation (the 3x3x3 supercell, with 1701 atoms): 9 days
- ▶ Wigner-Seitz scheme: 43 minutes
- ▶ Speedup: 300x

Ion Dynamics

- ▶ NEB with varying cell size, to simulate e.g. phase changes (see right)
- ▶ Support for meta-dynamics using PLUMED
- ▶ Performance improvements in MD from using HDF5 trajectory files
- ▶ Support for valence force fields (VFF) added
 - Automatic bonding assignment

Note: ATK-Classical has been renamed ATK-ForceField

New Builder Features

- ▶ Improved Wulff constructor - can now take multiple planes and contains a database of surface energies
- ▶ Measurement tool in the Builder and Viewer, also for NEB (dynamically updating with each image)
- ▶ Reorder atoms by drag and drop in the Coordinate List, or right-click to move to end/top
- ▶ “Send to” framework improved to remove any performance issues when handling millions of atoms in the entire workflow in VNL
- ▶ New GeneralizedLatticeMatch method for combining two arbitrary bulk crystal into an interface. The method is described in [Phys. Rev. B 96, 085306 \(2017\)](#).

New Analysis Features

- ▶ **Born effective charge analysis**
 - Enables geometry optimization and NEB in an applied electric field
- ▶ **Free energy analysis**
 - TotalEnergy now reports free energy and extrapolation to T=0 K
 - Zero-point energy and free lattice energy can be obtained from the PhononDensityOfStates analysis object (vibrational free energy in quasi-harmonic approximation of molecules and bulk)
- ▶ **Calculate and visualize Fermi surfaces**
- ▶ **Projections for DOS and band structure, project on atoms, shells, orbitals, spin**
- ▶ **Script for plotting spin textures**

Script Generator Updates (New Defaults)

- ▶ **SG15 Medium is now the default basis set**
- ▶ **Element and pseudopotential specific default mesh cut-off**
- ▶ **GGA-PBE is now the default exchange correlation**
- ▶ **The default electron temperature is now 1000 K (this is on the high side, to give better convergence; you may want to lower it for better accuracy)**
- ▶ **For devices, NeutralAtoms is now default**
 - Most systems will run a lot faster, in particular in parallel, and use significantly less memory
 - For some systems convergence can be worse, in which case the old default EquivalentBulk can be attempted
- ▶ **Adjusted the step length for elastic constants and relaxation to better suit DFT calculations**

Note: Due to these changes, the results from calculations run with “minimal scripts”, or by making a new script in VNL 2017, may differ from corresponding runs with 2016 and earlier versions

Job Manager Updates

- ▶ **New queue managers supported: LSF and SLURM**
- ▶ **Improved diagnostics tool**
- ▶ **Edit machines without need to delete existing jobs on it**
- ▶ **No need to save a file again, if using Send to from Script Generator**
- ▶ **Passwords and keys**
 - Built-in SSH key generation
 - Added possibility to store passwords in the Job Manager - removes the need to only do password-less ssh keys
- ▶ **Display the unique job ID to make it easier to identify the job**
- ▶ **Job ID made shorter, as some cluster place a character limitation on the job name in the queue**
- ▶ **Preview the PBS script**
- ▶ **Add custom lines to the submit script**
- ▶ **Use the PATH to locate the PBS binaries if the binary path field is empty (was earlier not permitted to leave this field empty)**
- ▶ **Special plugin for ATK On-Demand (Sabalcore)**

3D Plotting

- ▶ **Color atoms by computed quantities, like forces, velocities (see right), etc**
 - Also works in movies, e.g. MD trajectories
- ▶ **Repetitions**
 - Repetition of atoms can be synced with repetition of the cell
 - Device, repeat in Z visually
- ▶ **Isosurfaces**
 - Repeat synced with cell repeat
 - Chosen isovalue is now indicated on the colorbar
 - Solid color option
- ▶ **Easier control of multiple scene window (close all, close Viewer & all scenes)**
 - Scene list in Viewer for better overview
- ▶ **Easier to adjust position of colorbars**
- ▶ **Perspective projection also with shaders turned on**
- ▶ **Vector field plots for current density (see right)**

2D Plotting

- ▶ **New framework for 2D plots allows users to save and reuse customized plots**
- ▶ **Turns a 2D plot into a Python script, which can be modified or batch processed**
- ▶ **Combine plots, e.g. band structure and DOS**
- ▶ **Add annotations like arrows and labels to plots**

ATK-PlaneWave

ATK 2017 contains a preview of our upcoming plane-wave DFT module. For now, the performance is somewhat limited, but is already expected to change in a few months.

ATK-PlaneWave will set a new standard for DFT codes, as both beginners and experts will enjoy unsurpassed ease-of-use thanks to a complete integration in the graphical user interface for interactive setting up of structures and post-processing analysis and plotting, combined with powerful scripting capabilities via Python and database connectivity - i.e. just like for our LCAO-DFT code!

Platform Updates

- ▶ **ATK is now compiled against the Intel MPI library**
 - Automatic threading control in MKL for optimal hybrid parallelization - no need anymore to set OMP_NUM_THREADS for good parallel performance (unless you are doing an MD calculation with classical potentials)
 - Support for Infiniband
 - Intel's mpiexec.hydra is provided on Windows and Linux - this is the recommended way to run ATK in parallel
 - Maintained compatibility with MPICH2/3 and MVAPICH2
- ▶ **LM-X updated, same version on Windows and Linux**
- ▶ **Faster installation (esp. on Windows)**
- ▶ **32-bit platforms are no longer supported**
- ▶ **Mac OS X is no longer supported**

Miscellaneous

- ▶ Updated version of FHI-aims
- ▶ ABINIT removed from package
- ▶ Quantum Espresso plugins improved (bugs fixed), mainly required due to changes in the QE output file formats
- ▶ Surface configuration feature in a more mature state than in 2016. Reference: arxiv.org/abs/1707.02141.
- ▶ Log file improvements, less repeated information, more useful stuff
- ▶ Boykin's environmental tight-binding model implemented for strained GaAs and Si
- ▶ Convergence info saved on object, even the history, can be queried later and a calculation can be checked for convergence
- ▶ Visible in VNL too
- ▶ New occupation functions: Methfessel-Paxton, Gaussian, ColdSmearing
- ▶ Improvements to the geometry optimization algorithm when using "rigid body" constraints
- ▶ AKMC scripter support
- ▶ CrystalStructurePrediction polished and added to manual
- ▶ New Poisson solver: parallel conjugent gradient to replace MultiGrid and Direct solvers for systems with gates
- ▶ 2-9x faster than multigrid and uses 3-5x less memory unless you run in serial/few MPIs

Bugfix Update VNL-ATK 2017.2

Nov 02 2017

A bugfix update to VNL-ATK 2017 has been released (version 2017.2).

Download the update from <http://quantumwise.com/products/download> as usual. Your license for 2017.0 will work for this version too. For more information about VNL-ATK 2017, see the original release letter.

This update contains only a couple of fixed bugs and an updated EULA (End-User License Agreement) to reflect that QuantumWise is now part of Synopsys. Learn why QuantumWise becoming part of Synopsys is a big step forward for atomic scale modeling! (The number in parenthesis on each line is our internal tracking number.)

Fixed Bugs and Other Changes

- ▶ Added forgotten Effective Mass plugin (23481)
- ▶ Corrected the total energy in a LCAO spin-orbit calculation with `processes_per_kpoint > 1` (22862)
- ▶ ATK PlaneWave: BlochState only had periodic part, without phase (22772)
- ▶ Updated EULA to reflect that [QuantumWise is now part of Synopsys](#)

Sep 08 2017

A bugfix update to VNL-ATK 2017 has been released (version 2017.1).

Download the update from <http://quantumwise.com/products/download> as usual. Your license for 2017.0 will work for this version too. For more information about VNL-ATK 2017, see the original release letter.

This update contains a substantial amount of bug fixes, in particular several that fix various crashes. We are not aware of any bugs (solved or not) that would cause decidedly wrong results or errors in calculations (except very minor ones), but there were quite a few scenarios in which ATK 2017.0 would crash. The new 2D plot framework also received a touch-up in this release, and we spent some time solving minor annoying issues in VNL to improve the user experience. (The number in parenthesis on each line is our internal tracking number.)

Important Changes

- ▶ Two-center integrals are now calculated on a much finer grid. This gives improved accuracy for force forces and stress, which improves relaxations, phonon frequencies etc. It does, however, also mean that you might get slightly different results for these quantities in 2017.1 compared to 2017.0 and earlier (22476)
- ▶ New default PPS parameters for Ge, giving better band gaps (22745)
- ▶ Syntax and other errors now appear in stdout also when running in parallel, as was the case always before (22690)
- ▶ Warn, don't crash, if we fail to write a checkpoint file; also check if a checkpoint file can be written before the calculation starts (22107)

Added Functionality

We normally don't add any new features in updates, but some things were really missing in 2017.0, or we had strong requests from customers.

- ▶ Phonon bandstructure plot tool (existed in 2016, went missing in 2017.0) (22181)
- ▶ Added option Supercell tool deletes overlapping atoms (22186)
- ▶ Added the compound chemical formula to the last page of the Cleaver (20275)
- ▶ Enabled tag selection for MDTrajectories in the Viewer (22593)
- ▶ It is now possible to specify an "account" string in the PBS machine settings (22726)

Fixed Crashes

- ▶ VNL crashed (or at least does not display 3D graphics properly) showing GL_SCISSOR_TEST error messages (22177)
- ▶ Could not save DOS in HDF5 files when using 'save_partial=False' (22250)
- ▶ Spin-polarized LDA+1/2 was broken for devices/surfaces (22270)
- ▶ Viewer isosurface: +/- isosurface option was broken (22333)
- ▶ Using RandomSpin crashed when saving into HF5 file (22723)
- ▶ PW segmentation fault for Sn (SG15) (21762)
- ▶ Restarting PW calc with initial_state crashed when using MPI (22145)
- ▶ Don't crash if PYTHONSTARTUP is defined (and fails); appears to be common on OpenSUSE (22360)

Wrong Results Corrected

Although these issues could give wrong results, they are in reality small or would rarely appear in a real calculation.

- ▶ **Noncollinear GGA and MGGA gave slightly incorrect density in parallel (22718)**
- ▶ **Energies, forces and stress were wrong immediately after a DynamcialMatrix calculation using classical potentials (22061)**
- ▶ **Using integer occupation numbers in Slater-Koster gave wrong occupations in the density matrix (using floats worked fine) (22133)**
- ▶ **OptimizeGeometry with bonded force fields could return wrong connectivity (22163)**

Corrected and Improved Functionality

- ▶ Use caching to make the fat bandstructure plugin faster (22766)
- ▶ Default integral_lower_point was not updated in the Script Generator when changing pseudopotential (in 2017, this parameter is automatically adjusted to match the lowest eigenvalues of the specific pseudopotential used) (22265)
- ▶ Print forces smarter in the log file during relaxation, for easier grepping (grep for "OPT") (20027)
- ▶ Tag selection in Viewer is now active (22593)
- ▶ mpiexec messed up the license configuration when running in parallel on the local machine (22132)
- ▶ Calculating the mobility with just a single q-point failed (22152)
- ▶ IVCurve scripiter: "Self-energy calculator" drop-down menu was not functional (22252)
- ▶ Translate plugin stopped working for devices (22298)
- ▶ "Phonon energy intervals" method did not work with LOE (22376)
- ▶ Delete atoms in devices or surface could lead to index errors (22403, 22421)
- ▶ NEB did not set initial_spin correctly after reading (21951)
- ▶ Changing the fuzz factor would reset other graphical properties (21773)
- ▶ Error in Kerker preconditioner scripts (22272)
- ▶ Bad formatting of tags for 1000+ tagged atoms fixed (21878)
- ▶ NEB with only a start and a final (no interior) image failed (21921)
- ▶ PDOS crashed for molecules (22058)
- ▶ Improved error message when an error occurs while opening licenses.licconf (22096)
- ▶ Local machine in Job Manager: disabled threading options for serial jobs (22167)
- ▶ Choosing an electrode with a negative score (but same length as the actual "best" electrode) would make an error message appear in the Electrode Size plugin (22266)
- ▶ Isovalue indicator did not update for FermiSurface (22488)
- ▶ Plot2D issues
 - Dropping a graph drag icon on the toolbar was allowed and failed (21864)
 - Incompatible dimensions error could appear when arrow is present in a 2D plot (22659)
 - Made it possible to also annotate a 2D plot outside plot area (22059)
 - Plot interaction failed in logarithmic scaling (22325)
 - Ensure plt files can be dropped on the Editor (22050)
 - Fixed an issue with editing item properties on Windows (22628)
 - Made plot titles more consistent (22681)
 - Inconsistent legend for 2D plot after editing fixed (22060)
 - Arrow moves outside plot area in some case (22062)
 - Arrow handle could not be removed (22063)
 - It was possible to remove lines in the band structure analyzer (22680)
 - Overlay windows disappeared when changing the style in PDOS many times (22683)
 - Could not resize the internal parts of the PDOS analyzer on Windows (21991)
 - DOS and Bandstructure plot now use the same label fonts (22003)
 - An undesirable behavior in Color Selection could not be fixed, it's a Qt bug but a work-around is available (22679)
 - Could not measure in combined BS/DOS plot (22066)
 - Error when cancelling the creating of a combined BS/DOS plot (22067)
 - Fix an error with "scroll locked axis" and zooming (22514)

Updates to the FHI-aims Interface

- ▶ Electron density object was incorrectly processed in VNL (22083)
- ▶ "Internal" relaxation was wrongly scripted by Scriptor (22262)

Updates to the VASP Interface

- ▶ Fixed an issue with ordering of atoms when exporting NEB for VASP, by only sorting the atoms by element when they are not already in contiguous order (21778)

Platform-Specific Issues

- ▶ 2017 installer complains about icon generation at the end on some Linux distribution which are missing xdg-utils; the problem was harmless, but the installation appeared to fail (only the desktop icon would be missing) (22106)
- ▶ On Windows, the installer appears to fail when MSVC 2017 present - notably, VNL itself was correctly installed, just the Visual C++ runtime was not (and was not needed, since it exists already) (22477)
- ▶ The discontinued "chrome" cluster removed from the ATK On-Demand plugin (22388)

Documentation

- ▶ PhotoCurrent module added (22259)
- ▶ Description of how to use "metatext" in HDF5 files added (22537)
- ▶ The working name OneShotDisplacement is properly replaced with SpecialThermalDisplacement (22258)
- ▶ InGaN potential references was incomplete (22328)

Known Remaining Bugs

- ▶ Slightly wrong total energy in a LCAO spin-orbit calculation with processes_per_kpoint > 1. However, this only affects non-converged results, specifically if you just take 1 SCF step (22862)
- ▶ NEB calculation crashes with preoptimization=True if you set processes_per_neb_image=None (workaround: optimize the end-points before creating the NEB path - generally a good idea anyway) (22868)
- ▶ System fonts with incorrect permission crash matplotlib on startup. Not really something we are responsible for fixing... (workaround: make sure your fonts are all readable by all users) (22487)
- ▶ Unicode support is still patchy, there are some areas that still don't accept unicode characters (22760 and a few others)
- ▶ Back Engine Exception if NEB and HTST run in the same script (workaround: run them in separate scripts) (22698)
- ▶ FHI-aims hangs in ELPA solver with MPI (we have a workaround, contact support if you need it) (22907)
- ▶ Measure tool can be a bit jumpy in devices (22000)
- ▶ TransmissionEigenvalues cannot be nlsaved in parallel (22902)
- ▶ SLURM plugin does not correctly enable OpenMP threading (22899)
- ▶ ... and minor stuff



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