

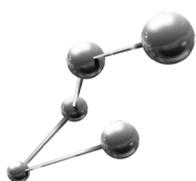
# ATK-VNL

## Release Features

### Version 2016

Last amended: June 2016

## ATK-VNL 2016



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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## Electron-Phonon Improvements

- ▶ Electron-phonon coupling is now also supported also for noncollinear/spin-orbit calculations
- ▶ General code optimization, giving about 10x better performance and reduced memory usage
- ▶ Generate energy-dependent scattering rates from the fully k-point dependent ones, for mobility calculations
  - A smallish approximation (often) which reduces computation time - and memory usage - substantially; cf. picture to the right
- ▶ All output is now in tensor form (conductivity/resistivity, mobility etc)
- ▶ New analysis options: First moment, Seebeck coefficient, thermal conductance (so, it's now possible to compute ZT with electron-phonon coupling included), Hall coefficient / Hall conductivity tensor
- ▶ New inelastic transmission spectrum (IETS) analyzer (cf. the analysis part of the tutorial on [IETS of a H-molecule between 1D Au chains](#) - this can now be done in the GUI, without scripts)

## General Performance Improvements

- ▶ Automatic multi-core parallelization per k-point - available already in 2015 but hard to use, now it's default which means ATK can scale out-of-the-box to 100s of cores even for systems with few k-points (cf. picture on the right)
- ▶ Improved performance of the LabFloor when project is located on a remote drive
- ▶ Multi-level MPI parallelization implemented for
  - HTST events
  - Adaptive Kinetic Monte Carlo (AKMC)
  - DynamicalMatrix computations
  - GlobalOptimization (aka crystal structure prediction tool)
  - IVCurve
  - Also fixed logging of these functions (all output now going to separate files)
  - For example, 3-level deep parallelization for AKMC (saddle searches, k-points, and multi-core per k-point) and similarly for DynamicalMatrix
- ▶ Improved parallelization of the contour integration in NEGF
- ▶ Brand new NEB implementation, a lot faster
- ▶ PEXSI solver
  - Order(N) for very (very!) large bulk systems
  - Can also be really useful for equivalent bulk (often a big bottleneck for devices)
  - Gamma point only and non-polarized, for now
  - Opens up for DFT calculations with 10,000+ atoms, as demonstrated by SIESTA (<http://arxiv.org/abs/1405.0194>) but requires parallelization over 100s or 1000s of cores
- ▶ Optimize forces and stress simultaneously, instead of leap-frogging stress/force steps as the old algorithm did, giving substantial improvements in calculation time (cf. picture on the right). Significant performance improvements in ATK-Classical (2-10x over 2015).
  - Benchmarks show that ATK-Classical is as fast as LAMMPS on a single machine (MPI is not yet implemented)

## New Basis Sets and Pseudopotentials

- ▶ Full set of SG15 pseudopotentials for the periodic table H-Bi (excl. the lanthanoids)
  - [Delta test](#) accuracy around 2 meV
  - Note: only available for GGA
  - Many with semicore states
  - Fully relativistic
  - Much softer than OMX or HGH
  - Medium/high/ultrahigh accuracy settings
  - [More information on the SG15 pseudopotentials](#)
- ▶ OMX basis sets have also been improved slightly

## Ion Dynamics & Molecular Dynamics (MD)

- ▶ **Entirely new MD framework in ATK**
  - All thermostats and barostats support linear heating and cooling
  - All barostats support both isotropic and anisotropic pressure coupling, as well as linear compression
  - All MD methods are improved wrt. stability, flexibility, and performance
  - Martyna–Tobias–Klein barostat, state-of-the-art algorithm, replaces the NPTMelchionna method
  - Corrections for some mistakes in the ASE MD routines
  - Allows for more flexibility to implement e.g. meta-dynamics
- ▶ **New constraints framework for MD and geometry optimization**
  - XYZ constraints added
  - Fix center of mass in MD
  - Can now constrain the Bravais lattice also when target stress is applied
  - New MD framework also allows implementation of custom constraints (example: implement a simple force field as a constraint)
- ▶ **Quick estimate of the HTST rate pre-factor using the curvature of the NEB reaction path**
- ▶ **Show warning (at beginning and end of simulation) if NEB end-points are not optimized**
- ▶ **New potential type in ATK-Classical**
  - MEAM: a very flexible potential type, that is applicable to both metallic and covalent systems

## OneProbe | SurfaceConfiguration

- ▶ **Brand new, revolutionizing concept - compute real surfaces without resorting to the slab approximation, but instead using an NEGF approach with real physical boundary conditions**
- ▶ **Calculate the surface properties of materials with more systematic convergence and effort (order of magnitude) than the slab approach**
- ▶ **Numerical contour integration of the surface Green's functions, coupled to DFT - i.e. just like for two-probe devices, but with only one electrode (the substrate)**
- ▶ **Properly describes charge transfer from bulk to surface/molecule (in a slab, moving charge to the surface leaves the "bulk" charged which shifts the Fermi level)**
- ▶ **Allows inclusion of real bias on surface, without dipole correction, which is particularly important for reaction barriers on surface**

### Example Applications:

- Work function calculations
- Molecular absorption
- Heterogeneous catalysis
- Surface reactions (MD, NEB)

## Script Generator Updates

- ▶ **Set MGGA-TB09 "c"-parameter**
- ▶ **Improved functionality in "Analysis from File"**
  - Read also DynamicalMatrix and HamiltonianDerivatives and other quantities
  - Query the NC file for available object IDs
- ▶ **Set solvent dielectric constant for the Poisson equation**
- ▶ **Set checkpoint file and time interval**
- ▶ **New constraints editor**
  - Also used for the DynamicalMatrix, etc.
- ▶ **Much more flexible approach for setting initial spins**
- ▶ **Setup of parallelization and other performance options**

## Job Manager Updates

- ▶ New diagnostics tool to help setting up remote clusters
- ▶ Possibility to set working directory for each job separately for remote jobs (still a unique subdirectory is created in the working directory)
- ▶ Many stability improvements

## 3D and 2D Plotting in VNL

- ▶ Autowrap atoms (outside the cell) in movies and other 3D windows
- ▶ Show equivalent atoms in bulk (periodically repeated)
- ▶ More flexibility for determining which atoms are bonded or not ("fuzz factor" control)
- ▶ Multiple light sources in 3D
- ▶ All 2D plots modernized, using Matplotlib
- ▶ New plot style for complex band structure plots, both in 2D and 3D
- ▶ Brillouin zone viewer, tooltips, and other improvements
- ▶ New volume rendering styles in 3D: voxel plots, point clouds (with carving options)
- ▶ Polyhedral view of crystals

## Plugins for External Codes

- ▶ New QuantumEspresso "Custom Scriptor" to generate QE input files
  - Also some added features for visualizing results
- ▶ VASP Scriptor updates
  - Set up constraints
  - Preview INCAR
  - Add your own custom lines to INCAR
- ▶ 20x faster LAMMPS import
- ▶ MBNExplorer import/export
- ▶ Cclib, for importing files from various quantum chemistry codes
- ▶ Packmol is now shipped as a plugin in the Builder, letting you set up initial structures for MD with molecules packed into a certain volume
- ▶ PyMatGen (pre-compiled) is now included in the package

## Licensing Updates

- ▶ Licenses that are checked out will never be checked in until the end of the script
  - This means, you will never end up in a situation where e.g. you are looping over DFT calculations, and the license is "stolen" by someone else midway in the script
- ▶ A parallel NEB calculation will now use only 1 master and N-1 slaves to run on N cores (earlier M masters where M=number of images).
  - Similar rules apply for AKMC, IVCurve, and other high-level parallel schemes
- ▶ Added command line parameter -X for faster start-up without auto-loading of the NanoLanguage module
- ▶ LM-X update to 4.8.1 for Linux
  - Fixes bugs in the license server scripts
- ▶ New license setup procedure, inside VNL
  - Guides the user, also when they have no license
  - Available from within VNL, to reconfigure the setup
  - More obvious how to obtain the "automatic" demo license
  - Much better error checking

## Platform Updates

- ▶ Mac OS X version introduced
- ▶ Better Unicode support: you can now name your project 日汉字
- ▶ RedHat/CentOS 5 are no longer supported
- ▶ libXC upgraded
- ▶ Switched from Qt4 to Qt5 - auto-solved some bugs and added new features in the API
- ▶ Still use PyQt4

## Miscellaneous

- ▶ Database tool to query the Crystallography Online Database
- ▶ Ozaki equilibrium contour; highly stable calculation of the equilibrium density matrix in device calculations, particularly useful if the electronic eigenvalue spectrum is very deep
- ▶ Verbosity framework, allows you to control how many details ATK should print out while running
- ▶ New k-point grids
  - Gamma-centered even Monkhorst-Pack k-point grids
  - General k-point shift also possible
  - Regular k-point mesh sampling for (Phonon)TransmissionSpectrum, including the edge of the Brillouin zone
  - Also added possibility to sample only a segment of the Brillouin zone
- ▶ Full Hartree potential can now be obtained
  - As a result, the old "ElectrostaticDifferencePotential" is now called "HartreeDifferencePotential" (unit eV)
  - ElectrostaticDifferencePotential and ElectrostaticPotential are now available with unit Volt (they are simply  $-1/e*\text{HartreePotential}$ )
- ▶ New "pseudopotential project shift" method - a semi-empirical way to tune the band gap of semiconductors and still obtain a good lattice constant (thus, a bit like Hubbard+U, but not self-consistent) which maintains possibility to optimize geometries (unlike with MGGA)
- ▶ New public methods for configurations, like setCartesianCoordinates (to move atoms)
- ▶ Added keyword Evac for DFTB, like in Hückel
- ▶ All correlation functionals and basis sets are now available for MGGA
- ▶ Icosahedron builder
- ▶ PhysicalQuantity engine radically improved
  - Avoid some annoying errors and allow more flexible notation, also allowing unit and unitless quantities to interact more easily
- ▶ Possibility to use different primitive-to-conventional transformation matrices
  - Also for UnitCell lattices
- ▶ VNL "crashlog" now pops up when generated, to give the user clear information about what went wrong

Mar 09 2017

A bugfix update to VNL-ATK 2016 has been released (version 2016.4). Download it from <http://quantumwise.com/products/download> as usual. For more information about VNL-ATK 2016, see the original release letter.

### Important Message

In order to make plots more consistent when dealing with atoms outside the unit cell, a new wrapping algorithm was implemented in ATK 2016.3. Unfortunately, this method is incompatible with calculations performed with older versions of ATK. That means, that if you “nload” the calculation from an older NC file (ran with 2016.2 or older) and compute e.g. the ElectrostaticDifferencePotential, the plot will appear to be incorrect. To avoid this, ATK 2016.4 will check if the calculation is old, and refuse to compute the grid data. The only way to work around this is to either rerun the calculation in ATK 2016.4, or use 2016.2 to compute the grid data. If you used 2016.3 for the calculation, you can safely use 2016.4 for post-processing. If, however, you use ATK 2016.3 for post-processing of files from 2016.2 or older, the data will be wrong (or appear to be, when plotted).

### Regular Bugs

- ▶ Thermoelectrics plugin corrected for spin-polarized cases (18686)
- ▶ Fixed error in nlsave when running an IVCurve with NoCheckpointHandler (18745)
- ▶ QuantumEspresso configuration reader updated for new QE file formats (18854)
- ▶ OpenBabel parser error fixed (18802)
- ▶ Corrected the behavior of polyhedra plots when hiding atoms (16419, 17158, 16564)
- ▶ Fix for thermostats not correctly dealing with constraints vs. thermalized groups (19660)

### Improvements and Additions

- ▶ Input fields which take a floating point number now accept both decimal points and commas more generally (17998)
- ▶ Added export of band data from the Bandstructure analyzer (18769)
- ▶ The “General Info” plugin now also supports SurfaceConfigurations (18397)
- ▶ Prevent VNL from being started as root when installer is run with sudo (18274)
- ▶ Some minor fixes to TremoloX, the ATK-Classical backengine

### Minor Fixes

- ▶ Fix crash that occurred when changing color maps in ProjectedLocalDensityOfStates (18409)
- ▶ Removed empty menus from the Crystal Builder (18929)



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