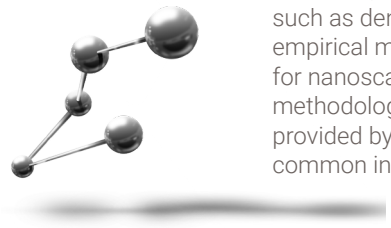
SYNOPSYS®

ATK-VNL Release Features
Version 12.8

Last amended: June 2012



ATK-VNL 12.8

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.

Important Note About Floating Licenses

If you have a floating license, you need to upgrade also the license server to LM-X 4.4, as ATK 12.8 will not work with LM-X license server version 3.6.3. The server packages are available from the download page.

Key Updates

- **Nudged Elastic Bands (NEB) - substantially upgraded functionality**
  - Improvements to the method itself (details are to be published separately)
  - Improved functionality for refining paths
  - Added capability to include gates in a NEB calculation
- **Complex Bandstructure**
  - Improved algorithm
  - Better reports/plotting
- **Piezoelectric tensor, based on Berry phase**
- **Noncollinear spin, both for bulk and devices (this feature is considered experimental; we are still working on making it possible to plot some of the computed noncollinear quantities, and optimizing some parts of the algorithms).**
- **New optimized basis sets**
  - Plus support for choosing (and plotting) them in VNL
- **Support for charged electrodes to simulate doping (already introduced in 12.2.2, but 12.8 includes a bug fix)**
- **VASP Scripter plugin updated**
  - Shipped with ATK 12.8, no need to install via add-on server
  - Better support for Hubbard U
- **Further improvements of the transmission spectrum calculation - we now set the transmission to exactly zero if there are no propagating modes. This should help distinguish a very low, but finite, transmission, from non-zero values due to numerical noise (basically, those values are now really zero).**

Other New or Updated Features

- **New Slater-Koster model for SiGe with a pair potential, intended for MD simulations [Shinomiya et. al, Memoirs of the Faculty of Engineering, Okayama University 35, 63 (2001)]**
- **Bandstructure can now be projected on atoms and angular momenta**
- **New shapes for metallic/dielectric regions: cylindrical and spherical (intended for wrap gates)**
- **ExchangeCorrelation potential analysis object**
- **MemoryUsage functionality - predict (to some level of accuracy) how much memory a calculation will require**
- **Updates to Mega-GGA, better handling of systems containing vacuum**
- **Progress bars for H0 - easier to see what goes on during the initial phase of a calculation**
- **Script Generator**
  - Enhanced selection of exchange correlation and Hubbard U
  - Added default ext ".py"
  - Can now drag script blocks between different open Scripters
- **Database touchups**
  - New molecule database with over 500 structures
  - Added some structures to the crystal database such as perovskites and several MoS2-type structures
- **Improved error messages when opening NC files from newer ATK versions**
- **Script with tags are now more compact**
- **More geometries added to the VNL examples directory**
- **Method to obtain the reciprocal unit cell vectors added to BulkConfiguration**
- **Update to LM-X version 4.4**
- **Effective Mass Analyzer plugin**
- **Installer now offers to launch license configuration tool**

Builder Plugins | New Functionality

- Interface Builder
  - More detailed control of lattice matching - enables building commensurate rotated layers and grain boundaries
  - Progress bar (Cancel button will come later)
  - Add layers at outside instead of at the interface
- Tag Editor - sorting issues solved
- “Keep Cartesian coordinates” is now default for Lattice Parameters
- Device from Bulk supports more systems and is more robust against weird cells
- Move tool now distinguishes 00-1 and 001 directions (useful for flipping systems)
- Supercell, clearer layout
- Nanowire plugin (like the Custom Builder in 11.8)
- Center now works for molecules too
- Almost all plugins updated cosmetically (incl. tab order)

Bugfix Update VNL-ATK 12.8.1

Fixed Bugs

- Fixed issue with NetCDF files that could become corrupted when they grew large. Also better handling for reading as much as possible from possibly corrupt files. If you have a corrupt NetCDF file which will not open in 12.8.0 (or in 12.8.1), we may be able to salvage it for you. Please contact support in this case.
- Lattice Parameters widget in the Builder was not always updated properly.
- Addon Manager, local install could fail, in particular on Linux.
- Move tool, “Fuse” operation removed too many atoms in a few cases.
- Bandstructure tick marks were incorrectly normalized. This did not affect actual results, only the relative distance between the symmetry points on the horizontal axis.
- Issues with Cerium basis set fixed.
- Undo made Coordinate List switch to Fractional.
- Supercell could rotate the cell, now keeps orientation. There was nothing wrong with the resulting structure before, but the new behavior is more convenient.
- Script Generator now supports all elements, also those without basis sets in ATK.
- Job Manager tooltip now properly shows location of output NetCDF files.
- VNL tutorial link in Help menu didn’t work.Movie threads were not stopped when window closed.
- Recursion is now the default self energy method everywhere. We recommend using it for most work.
- + a few more esoteric, small issues which you most likely would never notice.

Improvements and New Features

- Builder performance improvements for device structures.
- Improved mouse click selection to support users who click very fast (and thereby inadvertently draw a tiny rectangle, instead of clicking in a single point)!
- VASP Scripter improvements (import of VASP NEB paths to be published separately)
- Easier to identify when running in demo mode (or where license comes from).
- LM-X license server wrapper script (see the Installation Guide).
- New (experimental) plugin: POVRay – make ray-traced pictures of geometries

Bugfix Update VNL-ATK 12.8.2

A bug related to the license system has been discovered in 12.8.1. All customers using ATK 12.8.x must upgrade to ATK 12.8.2.

The bug is related to how ATK checks out licenses from a floating license servers for a device calculation. Normally only 1 master license is needed, but ATK 12.8.1 it checks out 2 master licenses.

The bug is not present in any earlier versions, but note that 12.8.0 has a few other small bugs that are fixed in 12.8.1 and of course also in 12.8.2.

In addition, an update to the Interface Builder plugin (versoin 1.4) is included ATK 12.8.2, but this can also be downloaded separately via the AddOn Manager.

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