

# NANOACADEMIC TECHNOLOGIES

Coherent Modeling

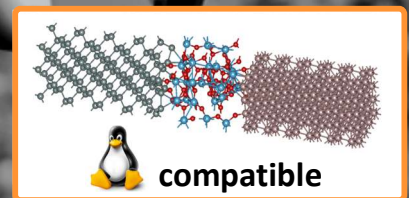
**Nanoacademic Technologies** develops advanced and innovative DFT-based solvers to study and predict materials and devices properties, as well as CAD tools for quantum computing technologies.

**NanoDCAL+** is an evolution of our state-of-the-art general-purpose first principles quantum transport package **NanoDCAL** – combining the nonequilibrium Green's functions (NEGF) formalism with density functional theory (DFT) – that predicts nonequilibrium quantum transport in nanostructures, including current-voltage characteristics of nanoscale devices and boasts new features, architecture and improved performance.



## A next generation multifunctional NEGF–DFT nanoelectronic transport solver

**NanoDCAL+** (**Nano** DFT **CAL**culator **plus**) is an LCAO implementation of NEGF–DFT. It is a general-purpose tool for ab initio modeling of non-equilibrium quantum transport. It inherits from **NanoDCAL** which has been used in hundreds of scientific publications in domains as varied as molecular electronics, nanotubes, topological insulators, batteries, magnetic tunnel junctions, metal grain boundaries and more. Its complementary set of features makes the best technological base for your R&D projects.



### Key features:

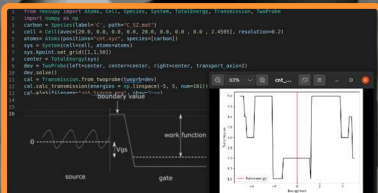
- Convenient Python API to efficient Fortran core
- Enhanced modularity and a brand-new GUI
- Improved parallelism, hardware portability and performance
- Focus on molecular and nanoscale electronics (realistic large-scale systems up to 10k+ atoms)
- Spintronics (collinear / non-collinear / spin-orbit coupling)
- Semiconductor nanoelectronics (I-V curve)
- Transmission, current and conductance calculators

Scattering states, photocurrents, thermoelectric currents, phonons calculations are part of **NanoDCAL** legacy version.

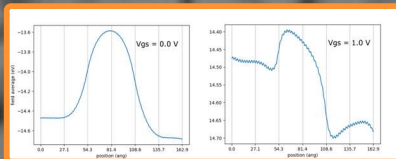
Updates and new versions are released on a regular basis and technical support is available to help our users by offering the best possible experience.

Stay tuned to our articles, newsletters and posts on our [LinkedIn](#) and [X](#) pages to avoid missing anything about Nanoacademic's latest news!

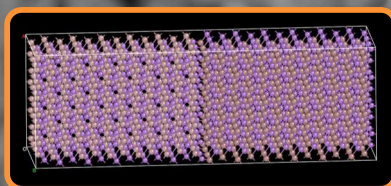
Contact us to test and adopt **NanoDCAL+**  
to catalyze your material studies and R&D projects!



Python API and plotting tools



Band diagrams and I–V curves



Quantum transport through  
molecules, 2D materials, and large  
atomic systems