NANOACADEMIC TECHNOLOGIES

Coherent Modeling

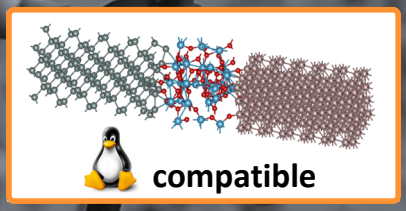
Nanoacademic Technologies develops advanced and innovative DFT-based solvers to study and predict materials and devices properties, as well as CAD tools for quantum computing technologies.

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.

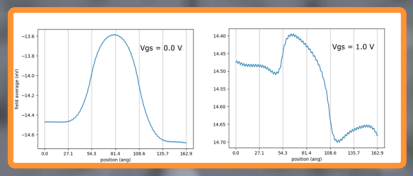
NanoDCAL

A next generation multifunctional NEGF–DFT nanoelectronic transport solver

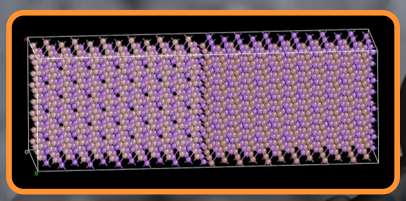
NanoDCAL+ (Nano DFT CALculator plus) is an LCAO implementation of NEGF–DFT. It is a general-purpose tool for ab initio modeling of non-equilibrium quantum transport. It inherits from NanoDCAL which has been used in hundreds of scientific publications in domains as varied as molecular electronics, nanotubes, 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.



Python API and plotting tools



Band diagrams and I–V curves



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

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!

DESIGN TOOLS FOR NEXT GEN MATERIALS

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