NANOACADEMIC TECHNOLOGIES

Coherent Modeling

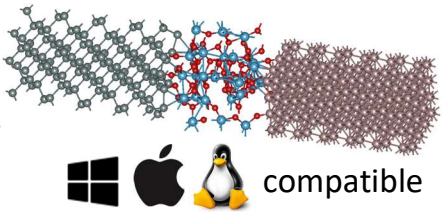
Nanoacademic Technologies distributes advanced and innovative DFT-based solvers to study and predict materials and devices properties, and computer-aided design tools for spin-qubits.

NanoDCAL is a state-of-the-art general-purpose first principles quantum transport package, 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.

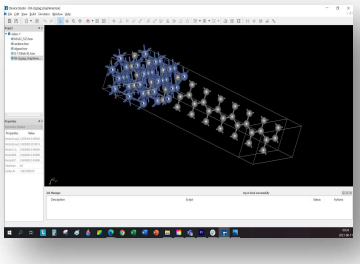
NANODCAL

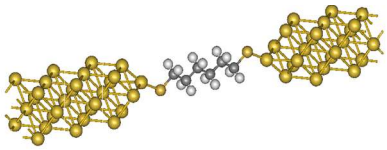
A multifunctional NEGF-DFT nanoelectronic transport solver

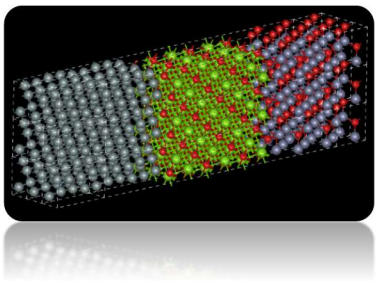
NanoDCAL (**Nano D**FT **CAL**culator) is an LCAO implementation of NEGF-DFT. It is a general-purpose tool for ab initio modeling of non-equilibrium quantum transport. It has been used in hundreds of scientific publications in domains as varied as molecular electronics, nanotubes, topological insulators, batteries, magnetic tunnel junctions, metal grain boundaries and more.



compatible







Key features:

- Written in MATLAB and C
- Focus on molecular and nanoscale electronics (small to large scale 1k+ atom systems)
- Spintronics (collinear / non-collinear / spin-orbit coupling)
- Semiconductor nanoelectronics (I-V curve)
- Several features such as total energy, force, scattering states and phonons calculations are part of NanoDCAL suite
- Study molecules, crystals, one-probe and two-probe systems
- Force, stress, structure optimization
- Electron-phonon coupling
- Atomic orbital basis optimizer
- Photocurrent
- Thermal transport coefficients

Updates 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 page 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!

+1 514-387-4003
nanoacademic.com
info@nanoacademic.com
666 Sherbrooke Street West, Suite 802
Montréal, Québec H3A 1E7 Canada