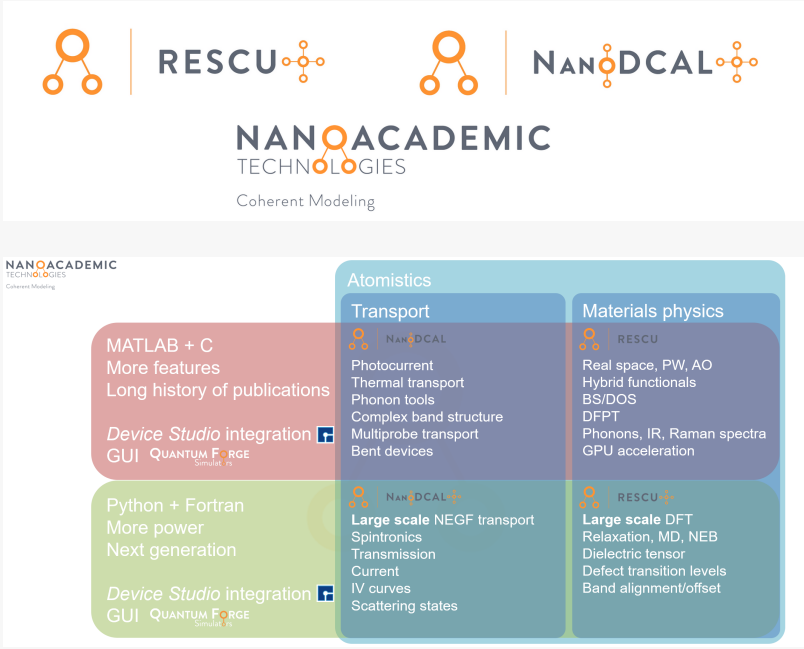
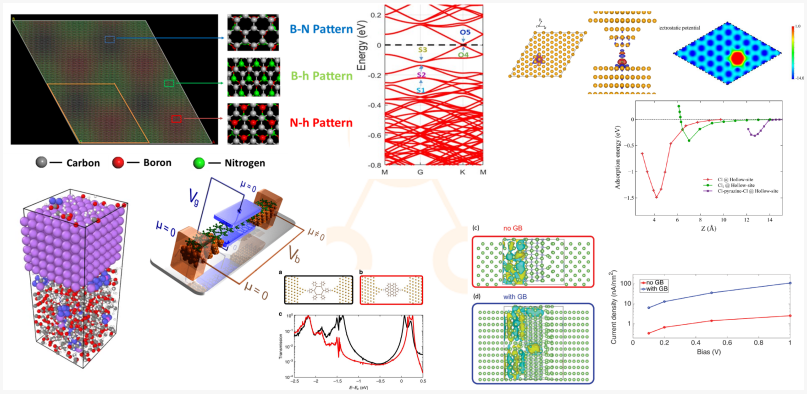
Advanced atomistic simulation: new build installation system to improve User experience - RESCU+ and NanoDCAL+

Release of a new version of some of the most advanced atomistic solutions on the market: RESCU+ & NanoDCAL+ (V2024.4.0). Build installation system is enhanced.

MONTREAL, QUEBEC, CANADA, April 22, 2024 /EINPresswire.com/ -- We are excited to release not only an updated version of the RESCU+ and NanoDCAL+ build installation system but a completely new one: this is part of version 2024.4.0 available for download on our User portal (https://portal.nanoacademic.com/).



Description of the main characteristics of Nanoacademic's atomistic software solutions



Some examples of atomistic simulations performed on different nanomaterials of interest

As described on our Documentation portal (See release note links below where tutorials, technological background, user manuals, etc), the installation process has been significantly enhanced to simplify the setup by our users and make sure that all dependencies and configurations are automatically handled for both our latest atomistic tool versions RESCU+ and NanoDCAL+.

RESCU+ and NanoDCAL+ are the improved versions written in Fortran of our legacy software RESCU for atomistic physics modeling and NanoDCAL for quantum transport simulation respectively.

But what are RESCU+ and NanoDCAL+ exactly ? *

RESCU+ (Real space Electronic Structure CalcUlator plus) is designed to offer a complete large-scale DFT solution. More specifically, it is an optimized, general-purpose Kohn–Sham DFT package including all the features listed below and more. It offers complementary features to its predecessor RESCU, such as AIMD and nudged elastic band method (NEB). With a convenient and easy-to-use Python API to an efficient and optimized Fortran core, plus a dedicated AI module (still under development in alpha phase), it offers better than ever parallelism and improved calculation times especially on clusters and supercomputers by at least one order of magnitude **. RESCU/RESCU+ are well fitted to study advanced materials and applications such as 2D nanomaterials (graphene + hBN and all sorts of heterostructures), Scanning Probe Microscopy (such as STM/AFM), optical properties, and more.

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/conductors, energy storage materials, magnetic tunnel junctions, metal grain boundaries (effects in batteries for example), spintronics and more. Its complementary set of features makes the best technological base for your material science R&D projects at atomic scale.

About the installation process, we knew this process was an uneasy path for non-expert users but now, it has become very convenient to setup and execute our atomistic software, feel free to test and see the difference as it runs and install automatically all the software files and dependencies.

V2024.4.0 release notes for more details:
RESCU+: https://docs.nanoacademic.com/rescuplus/releasenote_rescu.html#rescu-2024-4-0
NanoDCAL+: https://docs.nanoacademic.com/nanodcalplus/releasenote_nd.html

For more information about our advanced material simulation codes very well adapted to very large atomic systems, software brochures are linked below besides the full online documentation:
RESCU+: https://storage.googleapis.com/leaflets/Leaflet-RESCUplus_NanoacademicTech_v2023.pdf
NanoDCAL+: https://storage.googleapis.com/leaflets/Leaflet-NanoDCALplus_NanoacademicTech_v2023.pdf

Our main website has information on our other software solutions mentioned above as well as on QTCAD®, our unique on the marketplace spin-qubit modeling software for semiconductor-based quantum devices: online resources and more details can be found here: https://docs.nanoacademic.com/qtcad/.
There are QTCAD® users on 3 continents in companies and Universities designing the quantum

computers of tomorrow.

Please let us know any questions or comments, our expert team can be reached at info@nanoacademic.com

More to come soon as we plan to release another major user experience improvement later this year.

* These 2 pieces of software only support Linux based systems for now.
** Results based on several benchmarks performed on advanced HPC systems for very large atomic systems (10k+ atoms).

About Nanoacademic Technologies Inc.:
Nanoacademic Technologies Inc., established in Montreal since 2008, and with an office in the renowned Sherbrooke Innovation Zone, specializes in developing and licensing advanced atomistic simulation and quantum modeling software. Nanoacademic's software enables the prediction of properties and performance of next-generation materials and quantum devices. Utilized globally by universities, government labs, and private companies, Nanoacademic's software reduces development costs and time-to-market while unlocking new possibilities through powerful in-silico simulations.
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