NANOACADEMIC TECHNOLOGIES

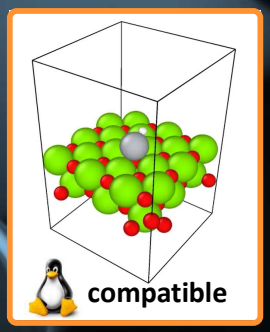
Coherent Modeling

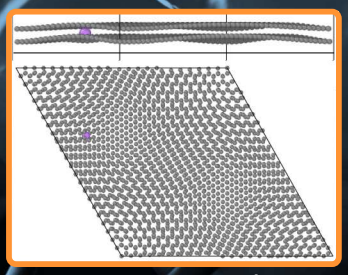
Nanoacademic Technologies develops advanced and innovative DFT-based solvers to study and predict materials and devices properties, as well as CAD tools for quantum computing technologies. Our powerful atomistic simulation tool RESCU+, with its new and improved design, offers a more powerful than ever set of features which enables simulating all atoms in a material using density functional theory (DFT) focusing on molecular dynamics (MD) and other ion dynamics. It also includes an innovative approach to such dynamics exploiting Machine Learning to provide drop-in acceleration to ab initio MD (AIMD) calculations.

RESCU+

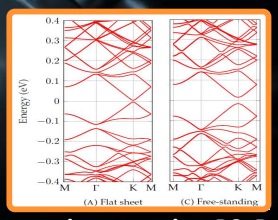
A next generation multifunctional large scale DFT solver

RESCU+ (**R**eal space **E**lectronic **S**tructure **C**alc**U**lator **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, it offers better than ever parallelism and improved calculation times especially on clusters and supercomputers by at least one order of magnitude *.

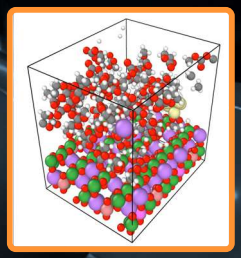




ML on bi-layer Graphene (2k+ atoms) and an intercalated Li atom



Electronic properties, BS, DoS



AIMD on bi-phase complex systems (Ex: energy storage materials)

Key features:

- Convenient Python API to efficient Fortran core
- Enhanced modularity and a brand-new GUI
- Improved parallelism, hardware portability, and performance
- Focus on very large atomistic systems up to 100k+ atoms
- Dipole moment, Mulliken populations
- Molecular dynamics, Machine Learning (AIMD/MLMD) (alpha versions)
- Structure relaxation, nudged elastic band
- Density, DOS/PDOS, LDOS, projected LDOS
- Band structures and unfolding
- Modeling of atomistic defects in materials
- Band alignment solver going beyond Anderson's rule
- Equation of states

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 try RESCU+
to catalyze your material studies and R&D projects!

DESIGN TOOLS FOR NEXT GEN MATERIALS

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* Based on benchmarks performed on Canadian cluster systems, 2000+ atom graphene-bilayer system