NANOACADEMIC TECHNOLOGIES

Coherent Modeling

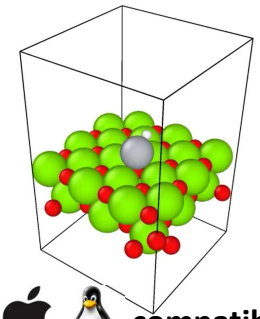
Nanoacademic Technologies develops advanced and innovative DFT-based solvers to study and predict materials and devices properties, and computer-aided design tools for spin-qubits.

Our powerful atomistic simulation **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 create 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 (NEB). With an enhanced modularity, a Python interface and a Fortran core, plus a dedicated artificial intelligence module, it offers better than ever parallelism and improved calculation times especially on clusters and supercomputers by at least one order of magnitude.



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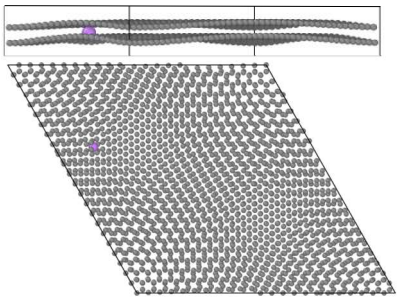

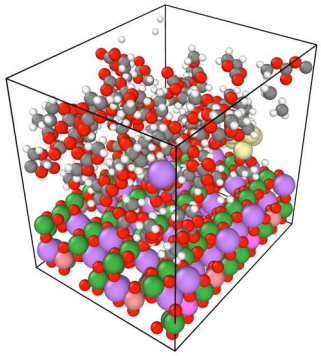

Key features:

- Written in Fortran and Python
- Provides enhanced modularity, interfaces with third party tools, improved parallelism, hardware portability and performance
- Focus on very large atomistic systems up to 100k+ atoms
- Dipole moment, Mulliken populations
- Molecular dynamics (AIMD/MLMD)
- Structure relaxation, nudged elastic band
- Density, DOS/PDOS, LDOS, projected LDOS, PLDOS
- Band structures and unfolding
- Defects tools
- Band alignment/offset tools
- Equation of states

Updates, 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 page 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!

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