**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.

compatible
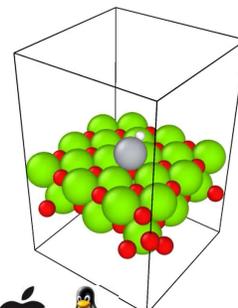
Key features:
- Written in Fortran and Python
- Provides enhanced modularity, interfaces with third party tools, improved parallelism, hardware portability and performance
- Focus on very large atomistic systems up to 100k+ atoms
- Dipole moment, Mulliken populations
- Molecular dynamics (AIMD/MLMD)
- 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
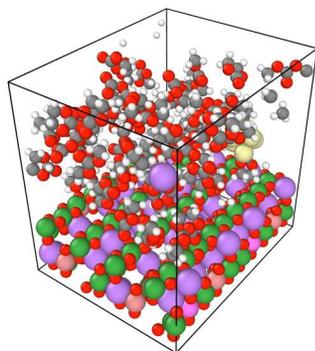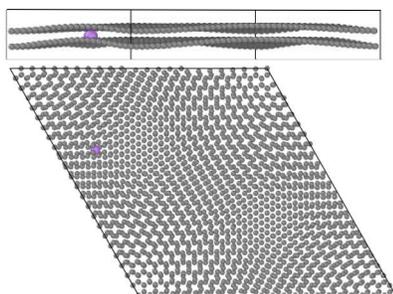
Updates, new versions are released on a regular basis and technical support is available to help our users by offering the best possible experience.

Stay tuned to our articles, newsletters and posts on our **Linked**in pages to avoid missing anything about Nanoacademic's and 4AM Software's latest news!

Contact **4AM Software** to test and try **RESCU+** to catalyze your material studies and R&D projects!

DESIGN TOOLS FOR NEXT GEN MATERIALS
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