NANOACADEMIC TECHNOLOGIES
Coherent Modeling

IN PARTNERSHIP WITH

4am Software
"where innovation meets infinity"

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 general applicability and predictive power, enables simulating all atoms in a material using density functional theory to solve the famous Schrödinger equation. It does so be discretizing the Kohn-Sham equation on real space grids, with plane-waves or with atomic orbitals. Its efficiency originates from numerical mathematics and parallel design and implementation.

RESCU

A multifunctional large scale DFT/DFPT solver

RESCU (**R**eal space **E**lectronic **S**tructure **C**alc**U**lator) is optimized to create a complete large scale DFT solution including a full set of features. More specifically, RESCU is a state-of-the-art general-purpose Kohn-Sham DFT package based on advanced numerical mathematics and a parallel implementation that can predict material properties on small computer clusters. It includes common electronic structure analysis tools and implements a perturbation theory extension of DFT (DFPT) which allows computing all sorts of response functions like polarization, phonon band structures or optical properties.
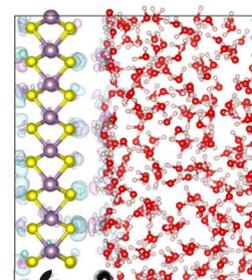
Key features:

- Written in MATLAB and C

compatible

- Focus on large scale systems (up to 20k atoms)
- DFPT implementation (e.g., dielectric tensor, dynamical matrix)
- Optical properties (e.g., dielectric permittivity, refractive index)
- Raman tools (e.g., tensor, spectrum, intensities)
- Advanced functional treatment such as DFT + EXX (hybrid) and DFT + U (Hubbard)
- Common analysis tools like DOS, PDOS, LDOS, PLDOS, band structure, band-unfolding, charge analysis
- Non-linear optical susceptibility
- Spintronics (collinear / non-collinear / SOC)
- Phonon tools (finite-difference-based)
- Large scale CFSI solver
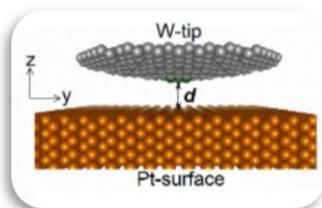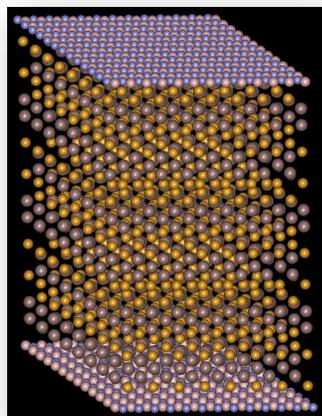
Updates, new versions are released on a regular basis and technical support is available to help our users by offering the best possible experience.

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!