NANOACADEMIC TECHNOLOGIES

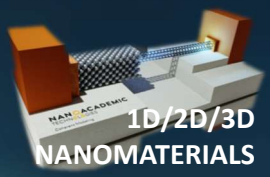
Coherent Modeling

Advanced Atomistic solvers for your Materials Science R&D Projects

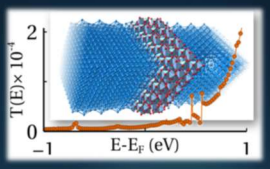
Nanoacademic develops state-of-the-art DFT solvers to characterize material properties and facilitate research into emerging materials. We offer software licenses consultancy services involving our most advanced simulation models: AI/ML, AIMD, very large atomic systems.

NanoDCAL (**Nano D**FT **CAL**culator) is an LCAO implementation of NEGF-DFT. It is a general-purpose tool for ab initio modeling of non-equilibrium quantum transport. It has been used in hundreds of scientific publications in domains as varied as molecular electronics, 2D/3D nanomaterials, nanotubes, topological insulators, batteries, magnetic tunnel junctions, metal grain boundaries and much more.

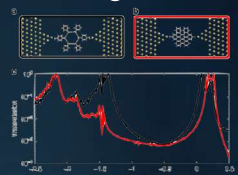
NANODCAL



1D/2D/3D NANOMATERIALS



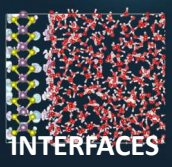
JOSEPHSON JUNCTIONS



I-V CHARACTERISTICS

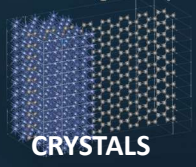
RESCU (**R**eal space **E**lectronic **S**tructure **CalcU**lator) is an optimized large scale DFT solver. More specifically, RESCU is a state-of-the-art general-purpose Kohn-Sham DFT package based on advanced numerical mathematics and a parallel implementation that can predict complex material properties on small computer clusters.
It implements a perturbation theory extension of DFT (DFPT) which allows computing all sorts of response functions like polarization, phonon band structures or optical properties among many other features.

RESCU

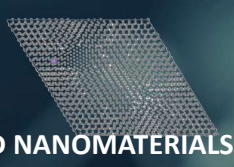


INTERFACES

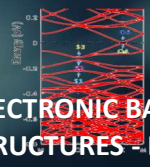
BATTERY MATERIALS



CRYSTALS



2D NANOMATERIALS



ELECTRONIC BAND STRUCTURES - DOS

Optimized computational resources: up to 1,000 atoms on a laptop! And 10k+ atoms on HPC

Our ***NEW Agentic DFT Simulation Assistant:*** LatticeMind

LatticeMind is an agentic pipeline where each module handles a specific part of the DFT simulation workflow to ensure accuracy, reproducibility, and reliability of your materials science R&D projects. It enables **faster onboarding** by lowering the entry barrier to RESCU and NanoDCAL, **reducing errors**, and **automating** structure setup, parameter tuning, and input generation.

LatticeMind

Workflow Generation
Creates complete RESCU & NanoDCAL workflows

Parameter Filling
Auto-fills structure, pseudopotentials, k-grids, SCF and XC parameters

Script Production
Bash job scripts + Python post-processing scripts

Materials Data Integration
Automatic retrieval with support for Materials Project

Tutorial-Style Reporting
PDF/HTML reports with detailed step by step instructions

RESCU NANODCAL & LatticeMind are now available on qBraid | LAB

- *No installation & No maintenance*
- *No HPC & DFT software configuration*
- *No queue + Efficient HPC*
- *Less troubleshooting & support*

account.qbraid.com

Setup-free cloud services layer

Users should review generated inputs and simulation parameters.

Single users, team/group licenses with **installation, HPC and support options**

Contact us to get a free trial license for our advanced atomistic and quantum tools then adopt it to catalyze your R&D projects!

Documentation Portal

User Portal to log-in

DESIGN TOOLS FOR NEXT GEN MATERIALS

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