Advance / NanoLabo

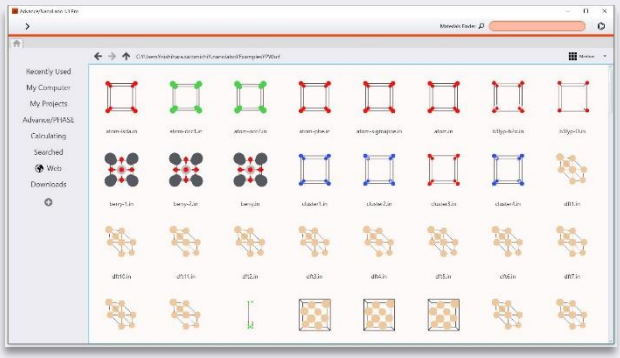
Developed by AdvanceSoft Corp. (2018 - 2024)
https://www.nanolabo.advancesoft.jp

Advance/NanoLabo

An integrated GUI capable of graphically operating various calculation solvers, including Quantum ESPRESSO*1, LAMMPS*2, and our product, Advance/PHASE. This interface simplifies setting modeling and calculation conditions by automatically searching for information in major materials databases such as the Materials Project*3. The results from these solvers are displayed graphically and instantaneously.

Features

- Iconic display of crystal structures (as shown on the right).
- Material database search via chemical formula input.
- Modeling for crystals, surfaces, interfaces, and molecules.
- Support for open-source calculation engines.
- Various visualization functions, including band structure, vibrational modes, reaction path afterimage display, kinematic animations, and more.



Functions

Modeling

Material database	Materials Project*3 PubChem*4
Crystal System	Cell Translation Supercell Impurity Substitution Lattice Defect Space Group Determination Primitive Cell Transformation Standard Cell Transformation
Surface & Interface System	Arbitrary Orientation of Surface Molecular Adsorption to Surface Mismatched Interface [Pro only]
Molecular System	Organic Molecule Illustration Solvent Molecule Filling Polymer Modeling [Pro only]

Calculation

Computational Engine	Advance/PHASE Quantum ESPRESSO*1 LAMMPS*2, ThreeBodyTB*5
Calculation Functions	SCF Calculations, Structural Optimization Hybrid Functionals, vdW Corrections Band Structure, Density of States (PDOS Calculator) Charge Density Visualization, etc. First-principles MD, Classical MD Thermal Conductivity, Viscosity Coefficients, Diffusion Coefficients TD-DFT, XAFS/EELS Phonon (Band Structure, Density of States) NEB Method, Work Function (ESM Method)
Computation Control	Job Scheduler NanoLabo-API for Python*6
Resources	Local Machine Compute Server (SSH Connection) Cloud

Operating Environment

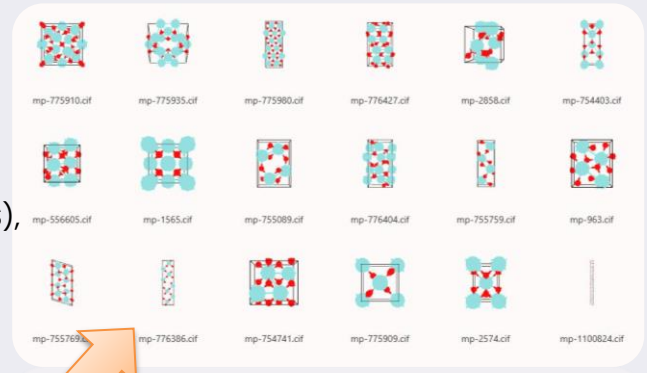
OS	- Windows 10/11 (64 bit) - AlmaLinux 8 (64 bit) - macOS 13 or higher (Intel/ARM64)
Machine Spec (Recommended)	CPU: Intel Core i7 or higher Memory: 10 GB or more

Online Manual

*1 Quantum ESPRESSO is a general-purpose open-source application for first-principles calculation, distributed under the GPL license. (https://www.quantum-espresso.org)
*2 LAMMPS is a general-purpose open-source application for classical molecular dynamics simulation, distributed under the GPL license. (https://lammps.sandia.gov)
*3 The Materials Project is a database for materials informatics developed at Lawrence Berkeley National Laboratory. (https://materialsproject.org)
*4 PubChem is a database for biochemistry developed at the National Center for Biotechnology Information. (https://pubchem.ncbi.nlm.nih.gov)
*5 ThreeBodyTB is an open-source application developed by NIST, designed for general-purpose tight binding methods. (https://pages.nist.gov/ThreeBodyTB.jl/)
*6 API specifications are available in the Advance/NanoLabo online manual. (https://nanolabo-doc.readthedocs.io/en/latest/python.html)

Modeling

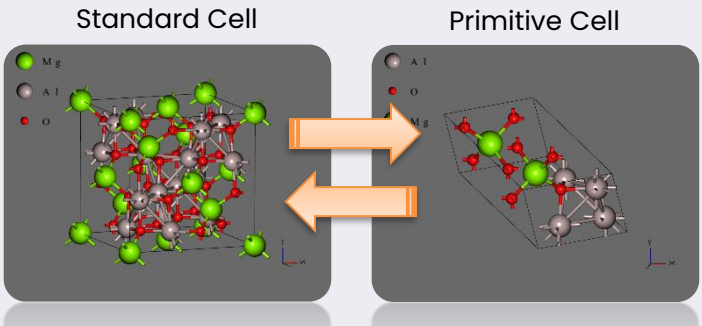
1. Material database



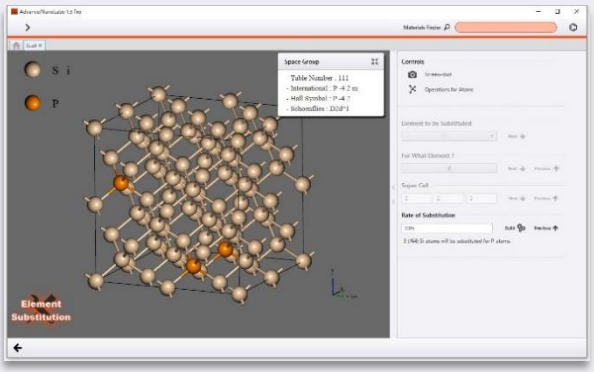
- ✓ Enter a chemical formula, molecular structure (SMILES), or molecule name into the search field to retrieve the corresponding crystal or molecular structure.
- ✓ Connect to the following databases via the Internet
  - Crystal structure： Materials Project
  - Molecular structure： PubChem

2. Crystal System

Spinel Transformation

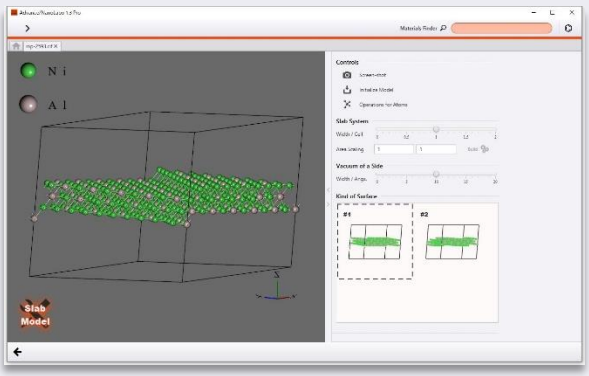


Impurity Substitution (P doping in Si)



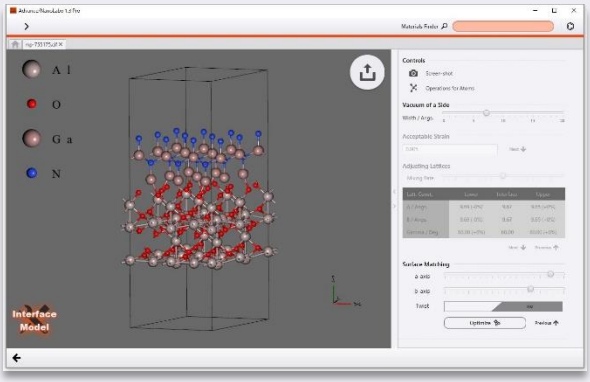
3. Surface & Interface System

Surface model (Ni_3Al [556]surface)



Using our original SlabGenom algorithm, arbitrary surface conditions can be generated.

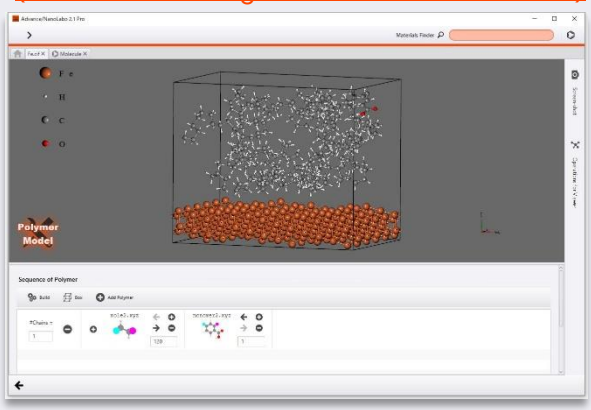
Interface model (Al_2O_3/GaN interface)



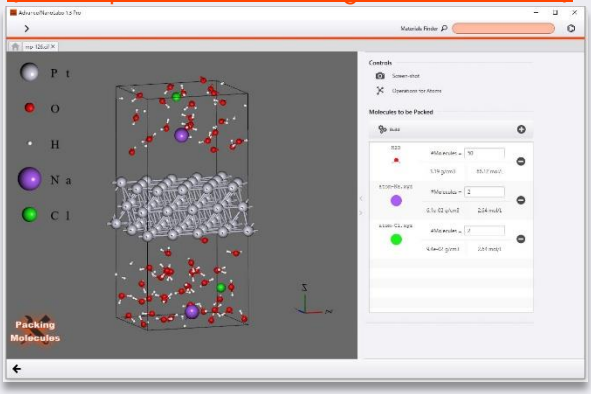
Lattice matching is achieved using the continuous fractional algorithm, which automatically optimizes the interplanar distances influenced by the classical molecular force field.

4. Molecular System

Polymer models (Enables interface generation with metal slabs)



Solvent molecular filling (NaCl aqueous solution filling around a Pt slab)



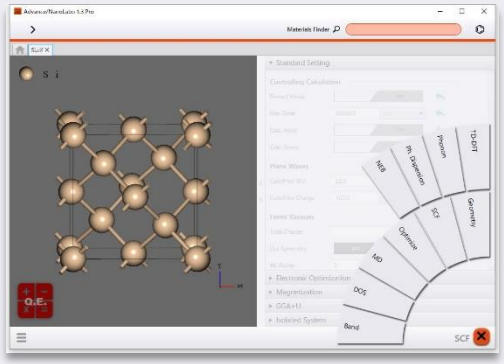
With our original packing algorithm, arbitrary solvent molecules and ions can be densely placed.

Calculation

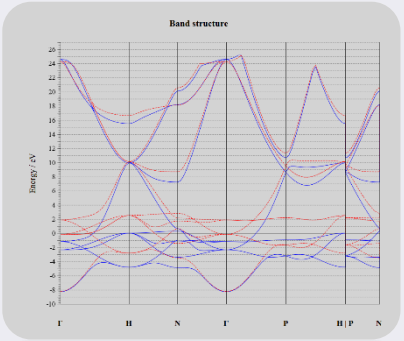
Quantum ESPRESSO

- ✓ Automatically generates appropriate input files directly from the crystal structure.
- ✓ Allows users to perform various calculations without the need for complex setting of conditions.
- ✓ Supports SCF calculations, structural optimization, band structure, density of states, ab initio MD, TD-DFT, phonon, and NEB methods.
- ✓ Visualizes the progress and results of calculations, with various types of post-processing available.

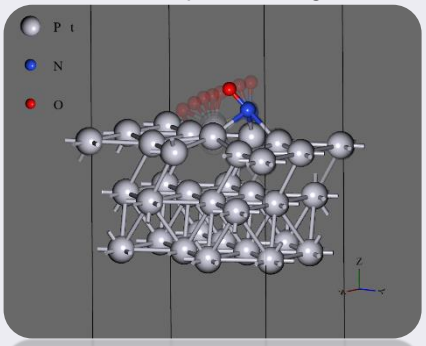
Input interface for Quantum ESPRESSO



Band structure plotting



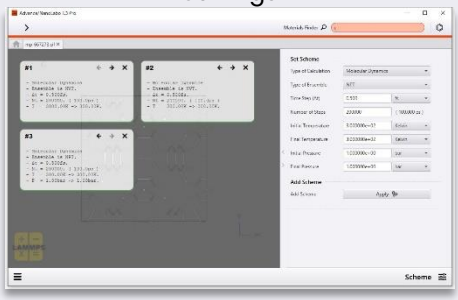
Visualization of the NEB Reaction Pathway Afterimage



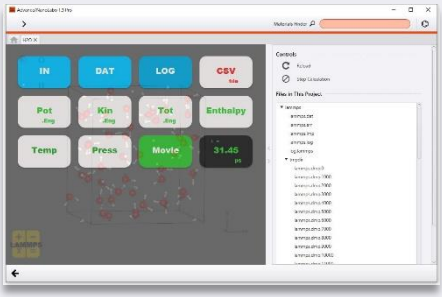
LAMMPS

- ✓ Supports Lennard-Jones, Charge, OPLS-AA, ReaxFF, Tersoff, EAM, MEAM, and Neural Network force fields*1.
- ✓ Allows setting multi-step calculation schemes (e.g., 100 ps motion in NVT ensemble, then switching to NPT ensemble).
- ✓ Displays animations of dynamics during calculations, with the option to save in MP4 format.
- ✓ External electric field, external force and translational movement for a given atom, and cell deformation. Visual definition of atomic groups.

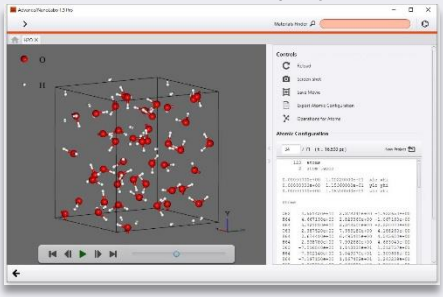
Multi-Step Calculation Scheme Settings



List of Calculation Items



Animation Display



*1 To utilize the Neural Network force field, our products, Advance/NeuralMD and the open-source Graph Neural Network force field, are available (for details, see the following page).

Computational Resources

Perform calculations on a local machine	- Calculation management via built-in job scheduler - Support for PBS, SLURM and PJM in the Linux version
Submit jobs to a computing server	- Execution of calculations on a Linux server via SSH connection - Job management using PBS, SLURM, or PJM

Using Cloud Services	- Science Cloud GPU*2
	  – bare-metal cloud environment provided by HPC Systems. (https://global.hpc.co.jp/)
	  – Submit jobs to the cloud from a local machine with NanoLabo installed.
	- Mat3ra*2
	  – SaaS cloud environment provided by Exabyte Inc. (https://www.mat3ra.com)
	  – NanoLabo is compatible with remote desktop on various platforms

*2 Additional charges are incurred for using cloud services.

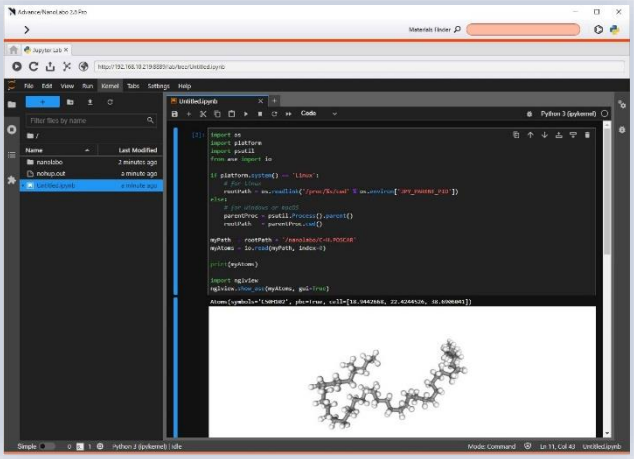
Graph Neural Network Potential

General-purpose Graph Neural Network force fields, compatible with a wide range of elements in the periodic table, are available. Specifically, **Open Catalyst**, **M3GNet**, and **CHGNet** are offered as open-source software options*1. All of these come with pre-trained models, eliminating the need for users to optimize the neural network themselves. This offers the advantage of enabling immediate molecular dynamics simulations for various systems. In addition, it is possible to load fine-tuned Graph Neural Network force field models or to operate Neural Network force fields created using our product, Advance/NeuralMD.

*1 Open Catalyst (https://github.com/Open-Catalyst-Project/ocp), M3GNet (https://github.com/materialsvirtuallab/matgl) and CHGNet (https://github.com/CederGroupHub/chgnet) are all implemented in Python, and they are designed to call these Python modules from LAMMPS to perform structure optimization calculations and molecular dynamics calculations.

Jupyter Interface for NanoLabo

This service enables the display and operation of Jupyter Lab*2 on the Advance/NanoLabo screen. It outputs Python code to create an Atoms object of ASE*3 by transferring the structure file, modeled in Advance/NanoLabo, to the server where Jupyter Lab is running. It is also feasible to integrate with **Matlantis** (https://matlantis.com), a general-purpose atomic-level simulation cloud service provided by Preferred Computational Chemistry Co., Ltd.



*2 Jupyter Lab (https://jupyter.org) is a web-based integrated development environment; however, here we primarily envision its operation as a Notebook with Python as the kernel.

*3 The Atomic Simulation Environment (ASE) is extensively used as a Python module for performing first-principles and molecular dynamics calculations.

Licensing

License Type

OS	License Type
Windows	Node Lock (Remote Desktop available)
Linux	Floating
macOS	Node Lock (Remote Desktop available)

License Price

Product	Annual (Business / National Institute)	Annual (Academic)	Permanent (Business / National Institute)	Permanent (Academic)
Advance/NanoLabo	500,000JPY*5	250,000JPY*5	1,500,000JPY*5	750,000JPY*5
Advance/NanoLabo Pro*4	900,000JPY*5	450,000JPY*5	2,700,000JPY*5	1,350,000JPY*5
Jupyter Interface	400,000JPY	200,000JPY	1,200,000JPY	600,000JPY

*4 Advance/NanoLabo Pro includes mismatched interface and polymer modeling functions.

*5 The license price is discounted when purchasing three or more units simultaneously. For more details, please contact our sales representative.

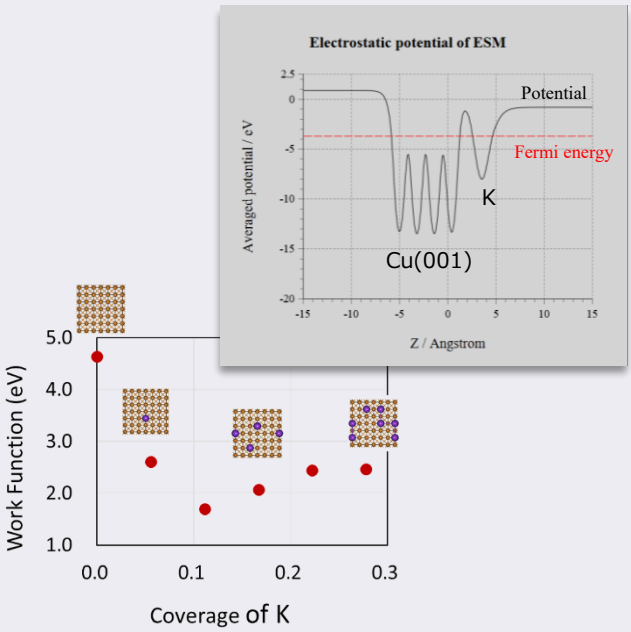
Trial licenses

Free trial licenses are available for one month per individual.

Cases

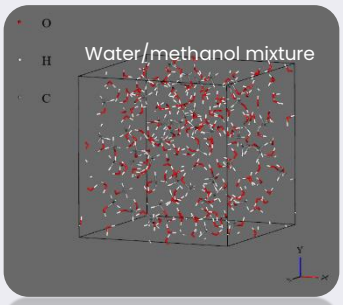
Work Function Calculation of K/Cu(001)System by ESM Method

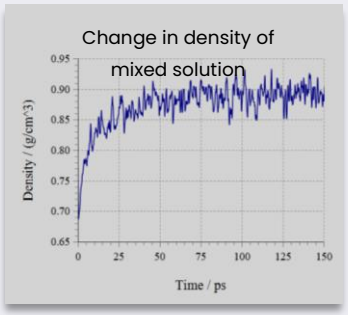
Using the Effective Screening Medium (ESM) method, the work functions of a Cu(001) surface with adsorbed potassium are calculated. This allows for the simulation of changes in the work function depending on the coverage ratio.



Calculation of Molecular Dynamics in Water/Methanol Mixtures

A model of a water/methanol mixture with a 1:1 volume ratio is developed, and molecular dynamics simulations are conducted using the NPT ensemble under standard temperature and pressure conditions (300K, 1bar). The OPLS-AA force field is utilized for molecular interactions.





Solution	Density (calculated)	Density (experimental)
Water	1.00 g/cm^3	1.00 g/cm^3 *1
Methanol	0.75 g/cm^3	0.79 g/cm^3 *1
Water/methanol	0.89 g/cm^3	0.93 g/cm^3 *2

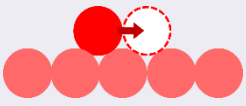
*1 S. Kim, et al: Nucleic Acids Res. 2019; 47(D1):D1102-1109.
*2 The Chemical Society of Japan (ed.): "Handbook of Chemistry, 5th Edition, Basic Edition II", Maruzen (2004) (in Japanese)

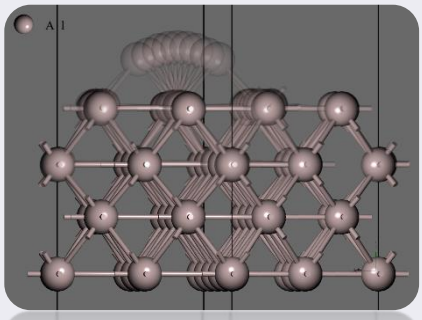
Analysis of Diffusion Pathways of Al Adatoms Using the NEB Method

Utilizing the Nudged Elastic Band (NEB) method, the diffusion process of adatoms on an Al(001) surface is analyzed. The activation energy is determined by calculating the two primary diffusion mechanisms: Hopping and Exchange.

Hopping diffusion

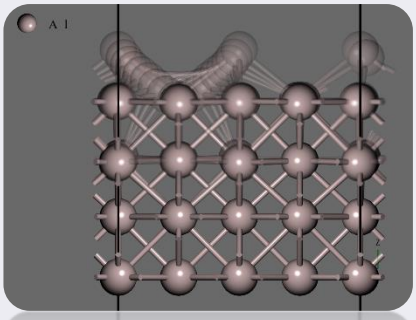
$E_a = 0.46$ eV





Exchange diffusion

$E_a = 0.14$ eV



AdvanceSoft Corporation

Please contact us first if you require additional information. Demonstrations can also be arranged.

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