Advance / NanoLabo

Developed by AdvanceSoft Corp. (2018-2021)

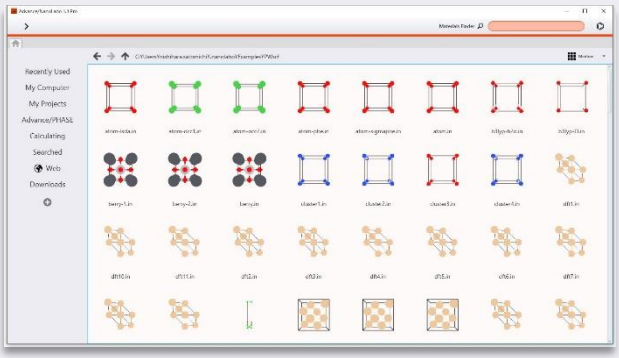
http://www.advancesoft.jp

Advance/NanoLabo

An integrated GUI which can graphically operates various calculation solvers such as Quantum ESPRESSO, LAMMPS. It is easy to set modeling and calculation conditions by automatically searching information in typical materials databases such as Materials Project. Results calculated by solvers are graphically displayed instantaneously.

Features

- Icon display of crystal structures (shown at right)
- Material database search by chemical formula input
- Modelling for crystals, surfaces, interfaces, and molecules
- Support for open source calculation engines
- Various visualization functions like band structure, vibration modes, reaction path afterimage display, kinematic animations, etc.



Functions

Modeling

Material database	Materials Project*3 PubChem*4
Crystalline	Cell translational movement Supercell Impurity replacement Lattice Defects Space group determination Primitive cell conversion Standard cell conversion
Surface・Interfaceline	Surface in any orientation Molecular adsorption on surfaces non-conformal interface [Pro only]
Molecularline	Drawing organic molecules Solvent molecular filling Polymer Models [Pro only]

Calculation

Computational Engine	Advance/PHASE Quantum ESPRESSO*1 LAMMPS*2
Calculation Functions	SCF calculation, structural optimization Hybrid functional, vdW correction Band structure, density of states (PDOS calculator) Visualization of charge density, etc. First principles MD, classical MD Thermal conductivity, Viscosity coefficient, Diffusion coefficient TD-DFT、XAFS/EELS Phonon (Band structure, Density of states) NEB method, Work Function (ESM method)
Computation Control	Job Scheduler NanoLabo-API for Python*5
Resources	Local machine Compute server (SSH connection) Cloud

Operating Environment

OS	- Windows 10 (64 bit) - CentOS 7 (64 bit) - macOS 10.15
Machine Spec (Recommended)	CPU: Intel Core i7 or higher Memory: 10 GB or more

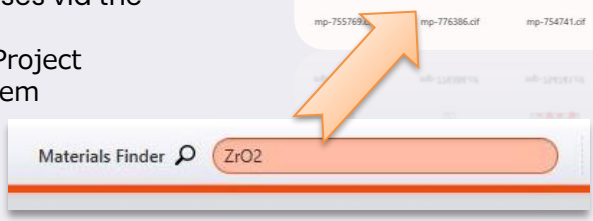
Online Manual

*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 API specifications are available in the Advance/NanoLabo online manual. (https://nanolabo-doc.readthedocs.io/ja/latest/python.html)

Modeling

1. Material database

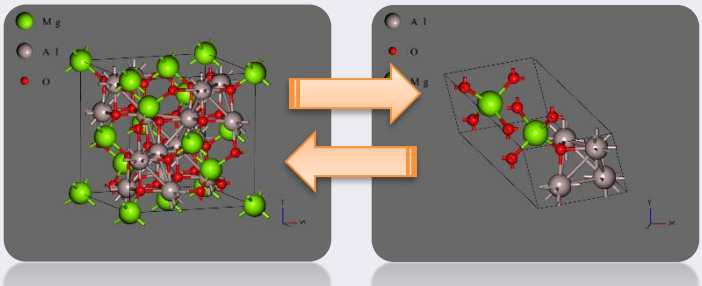
- ✓ Entering chemical formula or molecular structure (SMILES) or molecule name into the search field, you can get the crystal or molecular structure.
- ✓ Connect to the following databases via the Internet
  - Crystal structure： Materials Project
  - Molecular Structures： PubChem



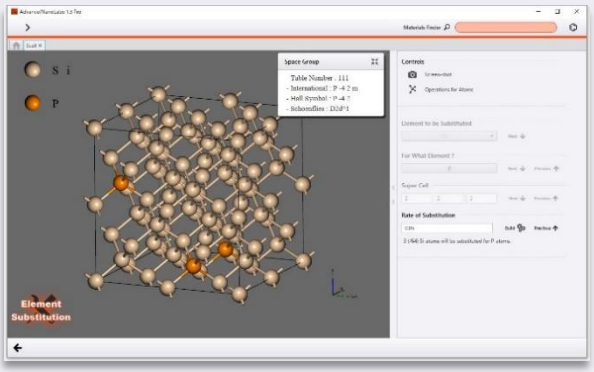
2. Crystalline

Cell conversion (spinel)

Standard Cell　　Primitive Cell

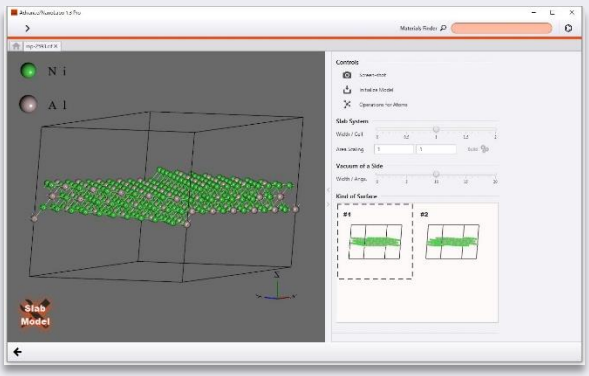


Impurity replacement (P doping on Si)



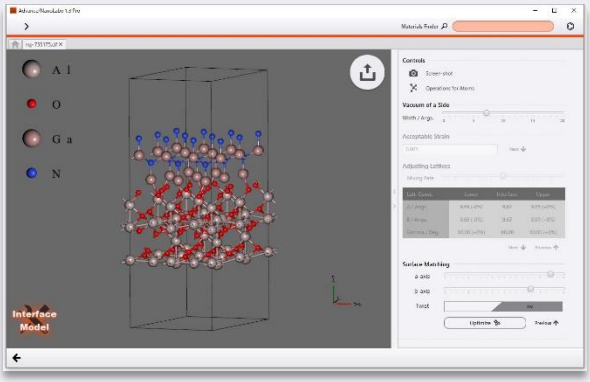
3. Surface・Interfaceline

Surface model (Ni_3Al [556]surface)



Based on our original SlabGenom algorithm
Arbitrary surface conditions can be generated.

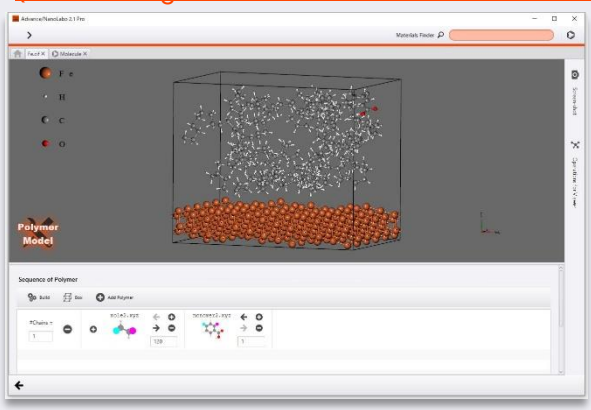
Interface model (Al_2O_3/GaN interface)



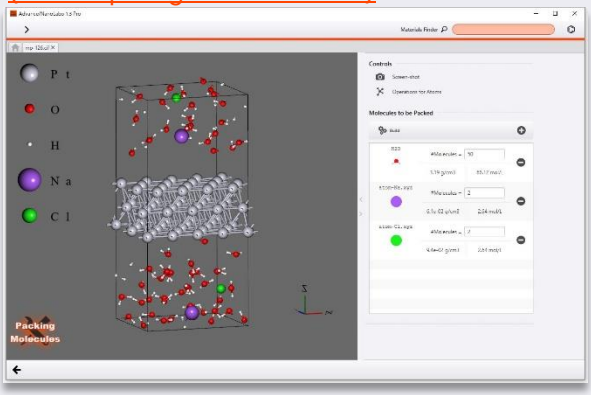
Lattice matching by the continuous fractional algorithm.
Automatically optimize the distance between planes caused by the classical molecular force field.

4. Molecularline

Polymer Models
(Possible to generate an interface with a metal slab)



Solvent molecular filling
(NaCl aq filling around Pt slab)



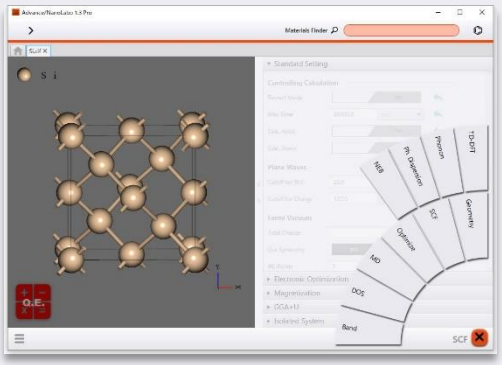
With our original packing algorithm, Arbitrary solvent molecules and ions can be placed in high density.

Calculation

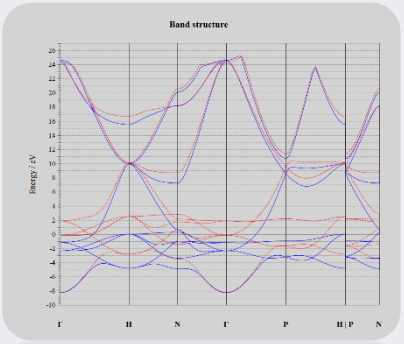
Quantum ESPRESSO

- ✓ Generate appropriate input files automatically, immediately from the crystal structure.
- ✓ Users can perform various calculations with no complicated setting of calculation 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. (Various types of post-processing are available)

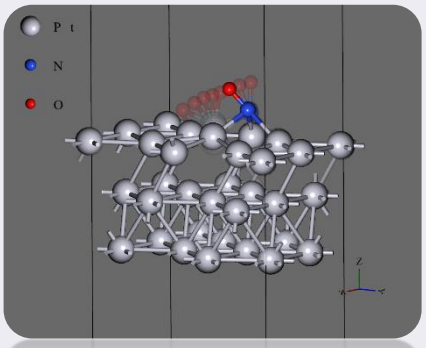
Input screen for Quantum ESPRESSO



Plot of band structure



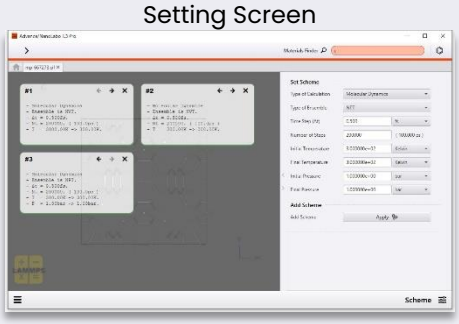
Cloned images of NEB reaction pathway



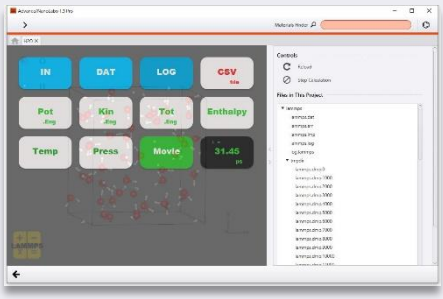
LAMMPS

- ✓ Supports Lennard-Jones, Charge, OPLS-AA, ReaxFF, Tersoff, EAM, MEAM, and Neural Network force fields*1.
- ✓ For organic molecules, the force field parameters of OPLS-AA are automatically assigned.
- ✓ Multi-step calculation scheme can be set. (e.g., 100 ps motion in NVT ensemble, then switch to NPT ensemble.)
- ✓ Displays animation of the dynamics even during the calculation. (Save as MP4 format)

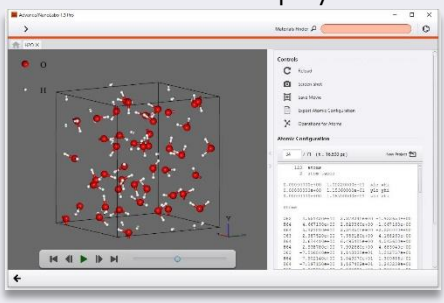
Multi Step Calculation Scheme Setting Screen



List of calculation items



Animation display



*1 To use the Neural Network force field, you will need to purchase Advance/NeuralMD separately.

Computational Resources

Run calculations on a local machine.	- Management of calculations with built-in job scheduler - Use of PBS and SLURM (Linux version only)
Submit jobs to compute server	- Run calculations on a Linux server via SSH connection - Job management by PBS and SLURM
Using Cloud Services	- Exabyte.io*2 – SaaS-type cloud environment provided by Exabyte Inc. (https://www.exabyte.io/) - NanoLabo can be used with remote desktop on the platforms.

*2 Additional fees apply for the use of cloud services.

Roadmap

Release schedule	version	Features to be implemented
2021/09	*2.2*	GIPAW (NMR spectral) *1 NeuralMD Interface enhancements
2021/12	*2.3*	Car-Parrinello Molecular dynamics
2022/2	*2.4*	Molecular Dynamics with state-of-the-art Graph Neural Network Potential developed by Facebook inc. *2
2022/summer	*2.5*	LAMMPS Interface enhancements Expansion of the available molecular force field Modulus of elasticity (stiffness tensor) *1
2023 -	*x.x*	NWChem Interface 3D-RISM／ESM-RISM*1 Calculation of thermodynamic quantities and phase diagrams *1 Alloy (cluster expansion method) *1 XPS spectrum*1 ...

*1 This feature is only available in Advance/NanoLabo Pro.
*2 Open Catalyst Project 2020 (https://opencatalystproject.org).

Licensing

License Type

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

License Price

Product	Annual (Company / National Institute)	Annual (Academic)	Permanent (Company / National Institute)	Permanent (Academic)
Advance/NanoLabo	500,000JPY*4	250,000JPY*4	1,500,000JPY*4	750,000JPY*4
Advance/NanoLabo Pro*3	900,000JPY*4	450,000JPY*4	2,700,000JPY*4	1,350,000JPY*4

*3 In Advance/NanoLabo Pro, mismatched interface and polymer modeling functions are available.
*4 License price can be reduced by purchasing 3 or more units at the same time. For details, please contact our sales representative.

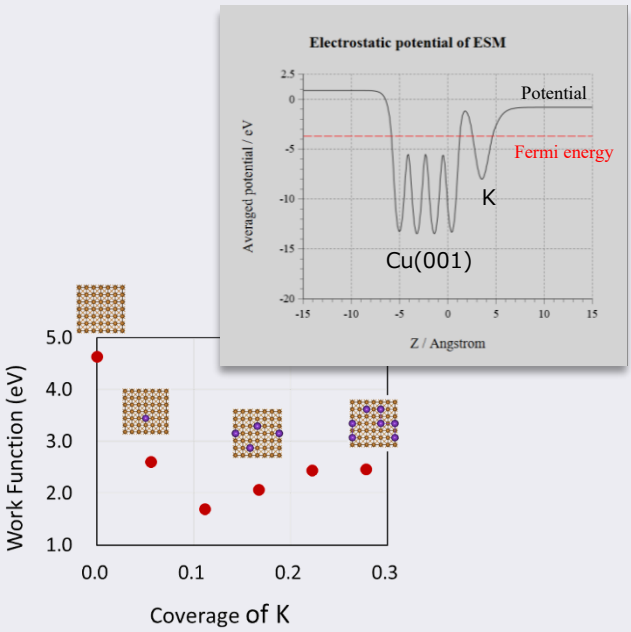
Trial licenses

Free trial licenses are available for one month per person.

Cases

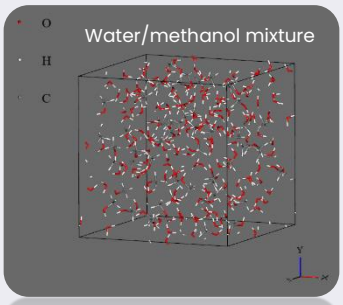
Work Function Calculation of K/Cu(001) System by ESM Method

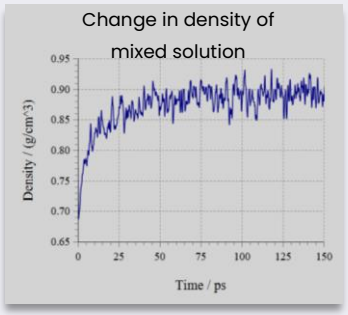
By using the Effective Screening Medium (ESM) method, the work functions on a Cu(001) surface with adsorbed potassium are calculated. The changes in the work function depending on the coating ratio can be simulated.



Calculation of molecular dynamics of water/methanol mixtures

A model of a water/methanol mixture (1:1 volume ratio) is created and molecular dynamics simulations are performed by the NPT ensemble under the condition of normal temperature and pressure (300K, 1bar). OPLS-AA is used for the molecular force field.





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

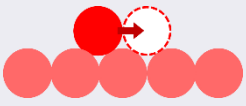
*1 S. Kim, et al: Nucleic Acids Res. 2019; 47(D1):D1102-1109.
*2 The Chemical Society of Japan (ed.): "Handbook of Chemistry, 5th Edition, Basic Edition II", Maruzen (2004) (in Japanese)

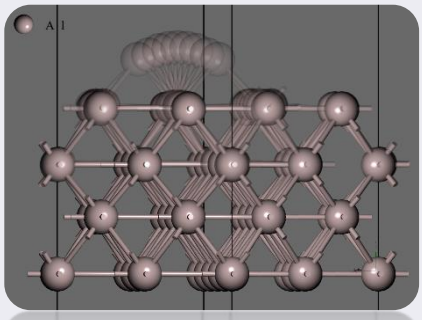
Analysis of Diffusion Path of Al Adatom by NEB Method

Using the NEB method, we have analyzed the diffusion process of adatom on Al(001) surface, and obtained the activation energy by calculating the two diffusion processes of Hopping and Exchange.

Hopping diffusion

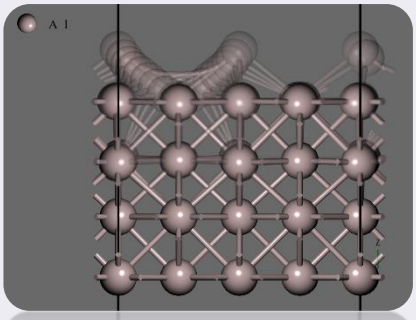
$E_a = 0.46$ eV





Exchange diffusion

$E_a = 0.14$ eV



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