# Advance / NanoLabo

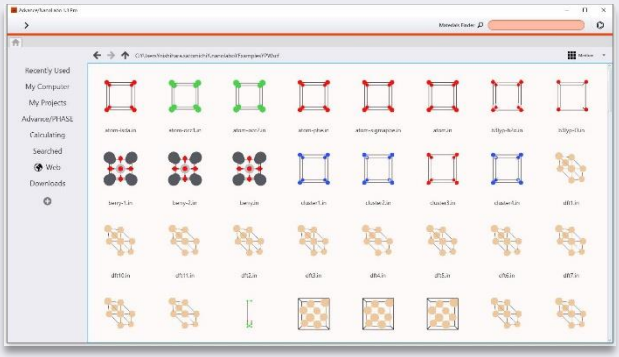
Developed by AdvanceSoft Corp. ( 2018 - 2024 )
https://www.nanolabo.advancesoft.jp

# Advance/NanoLabo

This GUI is compatible with open-source first-principles and molecular dynamics calculation software like Quantum ESPRESSO*1 and LAMMPS*2. It allows for extremely easy modeling and calculation condition setup by searching material databases such as the Materials Project*3. While enhancing convenience with generative AI, it also supports state-of-the-art Neural Network potentials.

## Features

- Iconic display of crystal structures (as shown on the right).
- Material database search with chemical formula.
- Gen-AI for modeling crystals, surfaces and molecules.
- Support for open-source calculation engines.
- State-of-the-art Neural Network potentials.
- Versatile visualization features for calculation results



## Functions

### *Modeling*

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

### *Calculation*

| | |
|---|---|
| **Calculation Engine** | Advance/PHASE<br>Quantum ESPRESSO*1<br>LAMMPS*2, ThreeBodyTB*5 |
| **Calculation Functions** | SCF Calculations, Structural Optimization, Hybrid Functionals, vdW Corrections, Band Structure, Density of States, Charge Density and Wave Functions Visualization, First-principles MD, Classical MD, Thermal Conductivity, Viscosity Coefficients, Diffusion Coefficients TD-DFT, XAFS/EELS, Phonon, NEB (Reaction Path), Work Function, Neural Network Potential |
| **Computation Control** | Job Scheduler<br>NanoLabo-API for Python*6 |
| **Resources** | Local Machine<br>Compute Server (SSH Connection)<br>Cloud |

## Operating Environment

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

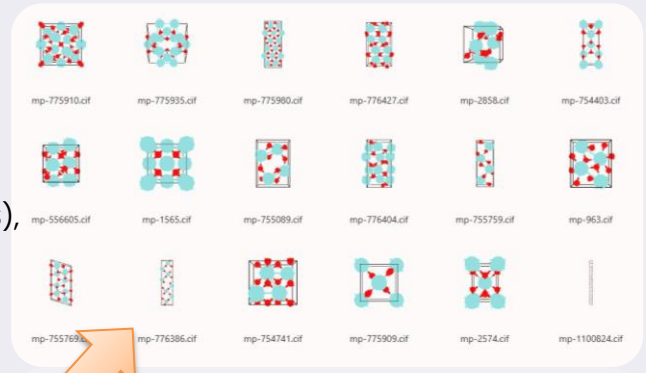
Demo of Advance/NanoLabo

*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

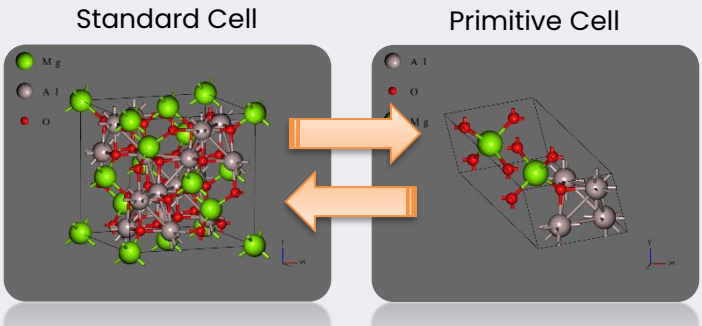
- ✓ Enter a chemical formula, molecular structure (SMILES), or molecule name into the search field to retrieve the corresponding crystal or molecular structure.
- ✓ Connect to the following databases via the Internet
  - Crystal structure： Materials Project
  - Molecular structure： PubChem



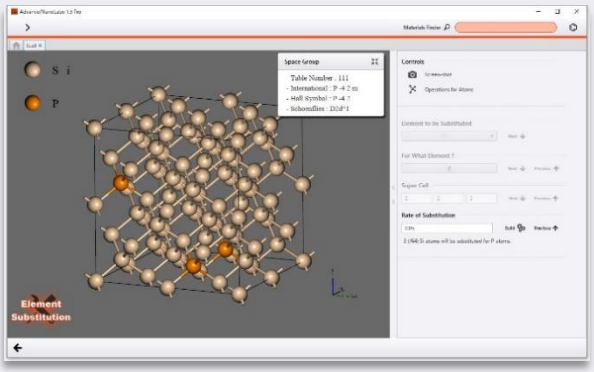


## 2. Crystal System

### Spinel Transformation

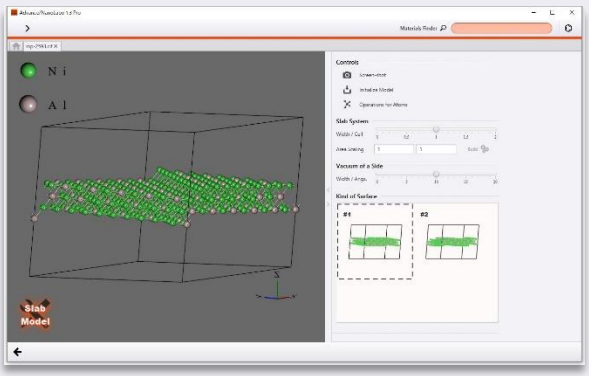



### Impurity Substitution (P doping in Si)



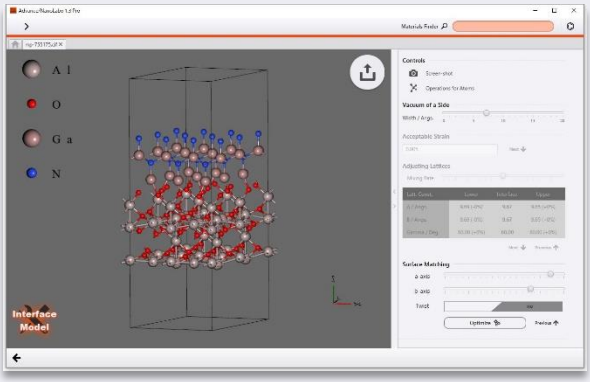

## 3. Surface & Interface System

### Surface model ($Ni_3Al$ [556]surface)




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

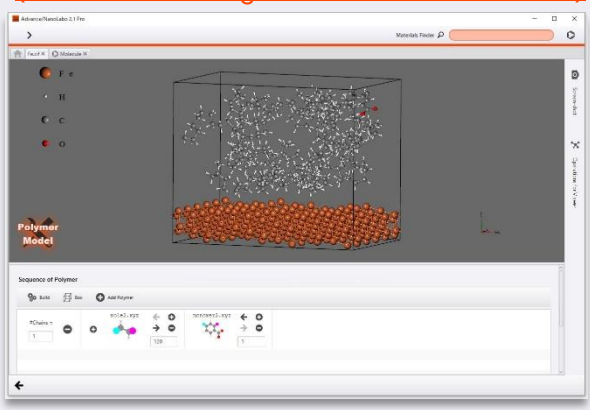
### Interface model ($Al_2O_3$/GaN interface)



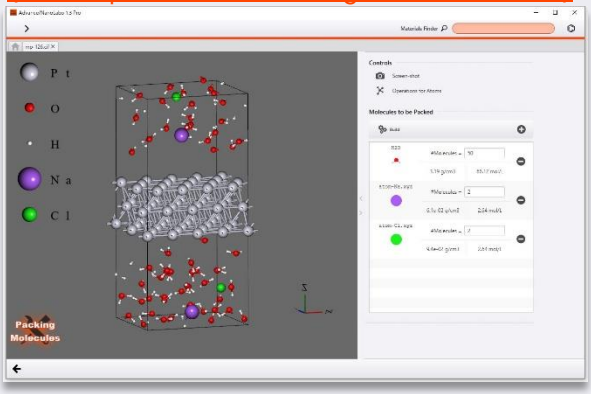

Lattice matching is achieved using the continuous fractional algorithm, which automatically optimizes the interplanar distances influenced by the classical molecular force field.

## 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.

# The world's first AI for generating material models.

I have pioneered the development of an Autopilot feature that automatically generates atomic structure models based solely on verbal input from the user. For example, models corresponding to the following command can be generated.

## 1) The solid-liquid interface between the 110 surface of an NMC electrode and a 1 mol/L LiBF4 solution in EC(7:3).

A supercell of layered LiCoO2 is created, and Co is substituted with Mn and Ni to form a (110) slab. Then, EC, DMC, Li+, and BF4- are packed in the specified ratios.
⇒ **The AI models the NMC electrode with an understanding of its meaning.**

## 2) An alloy of Fe/Ni/Cr/Mn = 7/1/1/1.

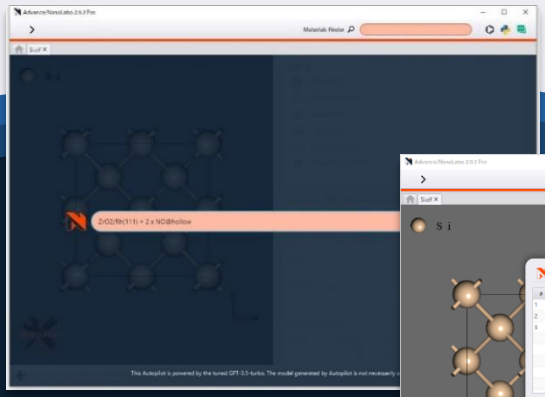
A supercell of Fe is created, then 10.0% of Fe is substituted with Ni, 11.1% of Fe is substituted with Cr, and 12.5% of Fe is substituted with Mn.
⇒ **The AI automatically calculates the element substitution rates.**

## 3) ZrO2(001)/Rh(111) + 2 x NO@hollow

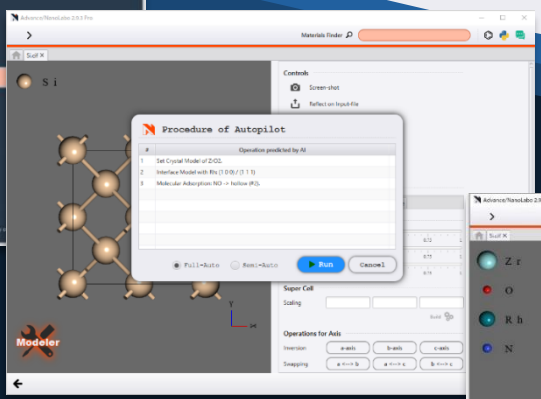
A model of the ZrO2 and Rh(111) interface is created, and two nitric oxide (NO) molecules are adsorbed onto the hollow site.
⇒ **The AI understands ambiguous expressions using chemical formulas.**

It also supports voice command input. Additionally, a "semi-auto mode" is available, allowing users to set details as needed while the AI performs automatic modeling. No additional costs will be incurred beyond the license fees for Advance/NanoLabo. The AI is implemented based on GPT-4o-mini. *1

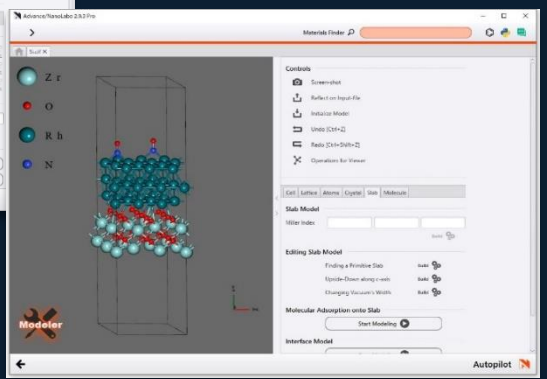
*1 The content entered by users is sent to OpenAI via servers managed by our company and processed by a large language model. The input information will not be used for the training of the large language model. Additionally, it will not be utilized in our product development unless the user agrees.



**1. input command with English**




**2. confirm procedure to generate the model**




**3. generate the model automatically**

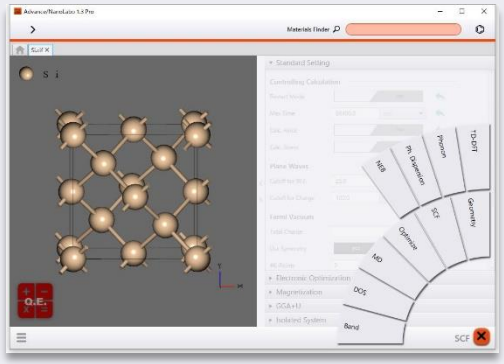
Demo of Autopilot

# Calculation

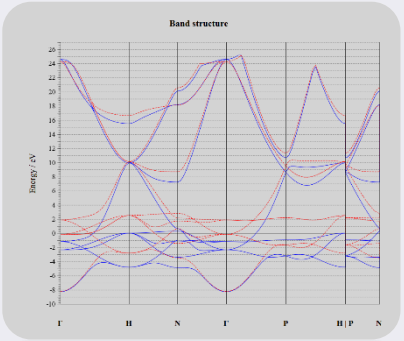
## Quantum ESPRESSO

- ✓ 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.

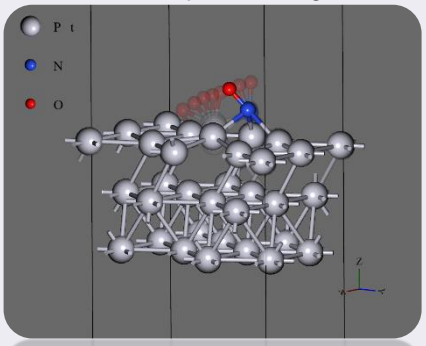
Input interface for Quantum ESPRESSO



Band structure plotting



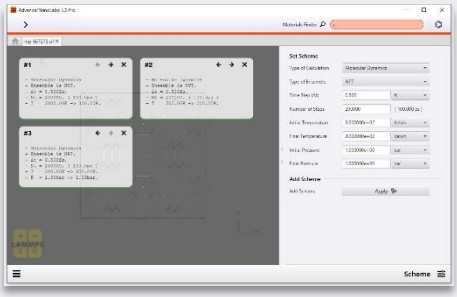

Visualization of the NEB Reaction Pathway Afterimage



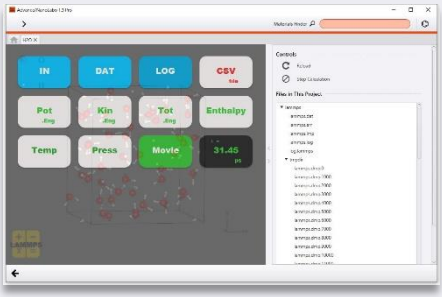

## LAMMPS

- ✓ Supports Lennard-Jones, Charge, OPLS-AA, ReaxFF, Tersoff, EAM, MEAM, and Neural Network potentials*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.

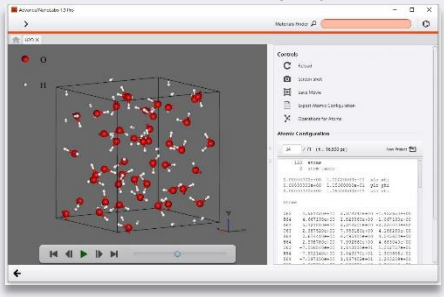
Multi-Step Calculation Scheme



List of Calculation Items




Animation Display



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

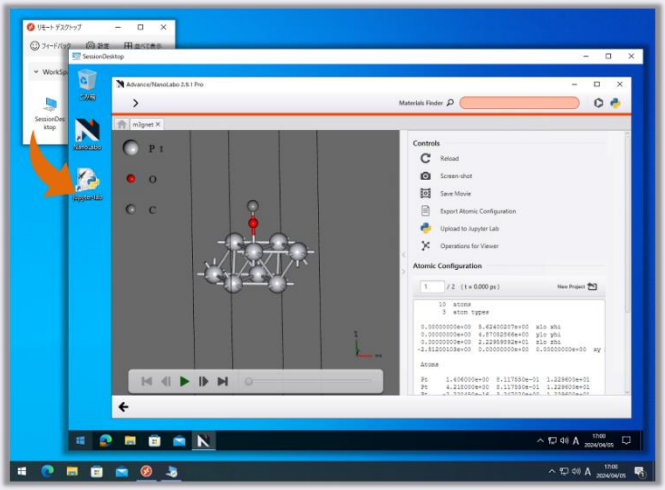
## Computational Resources

| | |
|---|---|
| **Perform calculations on a local machine** | - Calculation management via built-in job scheduler<br>- 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<br>- Job management using PBS, SLURM, or PJM |
| **Using Cloud Services** | - Science Cloud GPU*2<br>  – bare-metal cloud environment provided by HPC Systems. (https://global.hpc.co.jp/)<br>- Mat3ra*2<br>  – SaaS cloud environment provided by Exabyte Inc. (https://www.mat3ra.com)<br>- NanoLabo Cloud Desktop<br>  – virtual desktop on cloud, where Advance/NanoLabo works. (see the next page) |

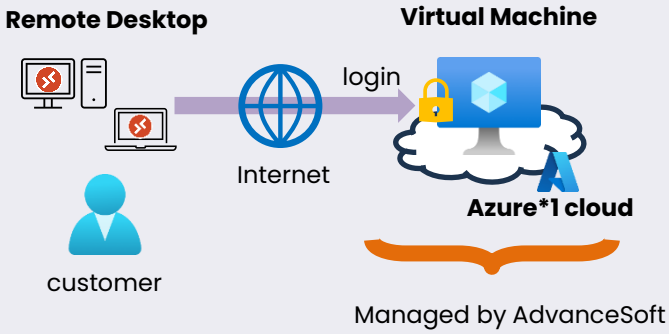
*2 Additional charges are incurred for using cloud services.

# NanoLabo Cloud Desktop

It is a subscription-based service that allows you to use the materials simulator Advance/NanoLabo in a cloud-based desktop environment. We provide a user-friendly GUI that is well-regarded, along with workstation-level computing resources. The necessary Python environment, including Graph Neural Network potentials, is pre-installed, allowing you to start computations immediately. The cloud environment utilizes Microsoft Azure Virtual Desktop, with management handled by Advance Software. Customers can simply connect via remote desktop without needing to worry about the cloud infrastructure.



## system overview diagram




## Comparison with Workstations and SaaS

| | Workstation | NanoLabo Cloud Desktop | SaaS |
|---|---|---|---|
| **Hardware** | Requires procurement and installation | Not required | Not required |
| **Software** | Software installation required | Pre-installed | Pre-installed |
| **Cost/Usage fee** | Costs for operation and maintenance | Fixed usage fee | Pay-as-you-go, etc. |
| **Interface** | Desktop environment | Desktop environment | Browser (custom UI) |

The convenience of the cloud and the usability as workstation.

## Specifications and Usage Fees

| | CPU cores | Memory | Strage | Usage Fee*2 |
|---|---|---|---|---|
| **Lite** | 8 | 32GB | 200GB | 450,000 JPY/year～ |
| **Regular** | 16 | 64GB | 400GB | 900,000 JPY/year～ |
| **Customization** | We will provide a quote based on your specified specifications. | | | |

Service introduction

*1 Windows and Azure are Microsoft products. © Copyright 2021 Microsoft Corporation. All rights reserved.

*2 The usage fees for Azure Cloud and the licensing fees for Windows are included, and there are no additional payments required from the customer to Microsoft. The license fees for Advance/NanoLabo are not included. The usage period is on an annual basis, and the specifications cannot be changed during the usage period.

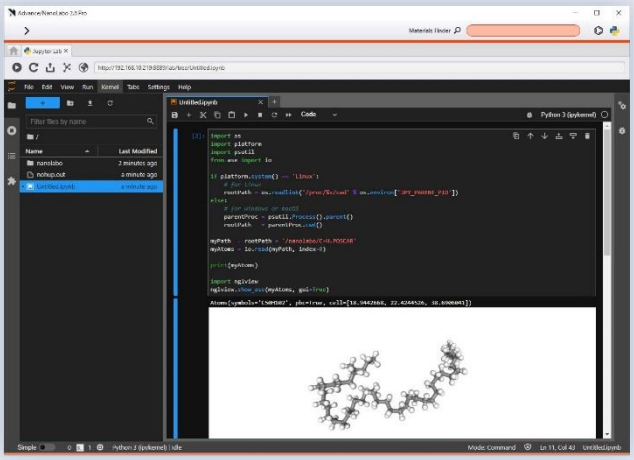
# Graph Neural Network Potential

General-purpose Graph Neural Network potentials, compatible with a wide range of elements in the periodic table, are available. Specifically, **Open Catalyst**, **M3GNet**, **CHGNet** and **SevenNet** 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 potential models or to operate Neural Network potentials 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. SevenNet (https://github.com/MDIL-SNU/SevenNet) is only compatible with Linux environments equipped with multiple GPUs.

# 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.

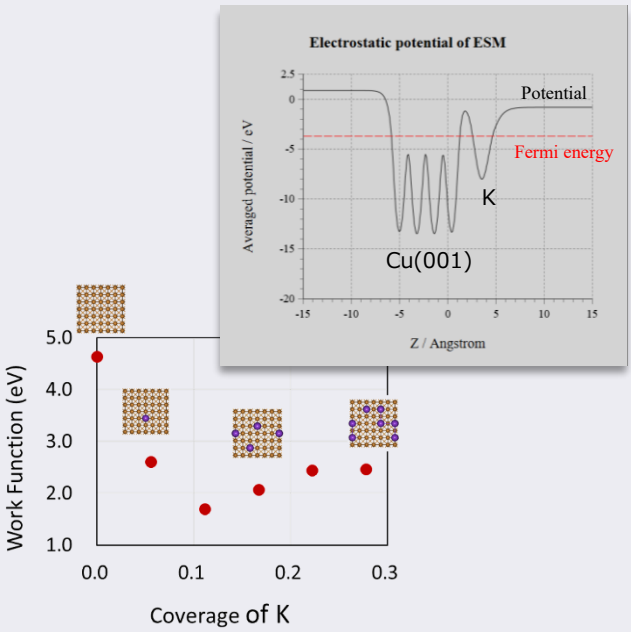
## Trial licenses

Free trial licenses are available for one month per individual.

# Cases

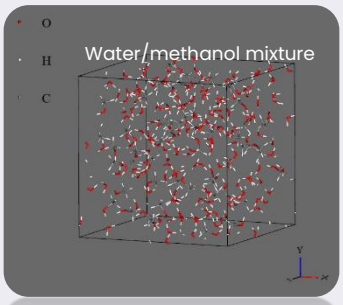
## Work Function Calculation of K/Cu(001)System by ESM Method

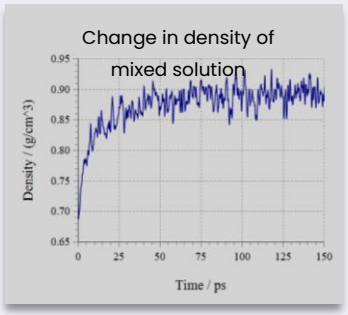
Using the Effective Screening Medium (ESM) method, the work functions of a Cu(001) surface with adsorbed potassium are calculated. This allows for the simulation of changes in the work function depending on the coverage ratio.




## 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 |

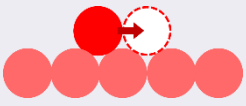
*1 S. Kim, et al: Nucleic Acids Res. 2019; 47(D1):D1102-1109.
*2 The Chemical Society of Japan (ed.): "Handbook of Chemistry, 5th Edition, Basic Edition II", Maruzen (2004) (in Japanese)

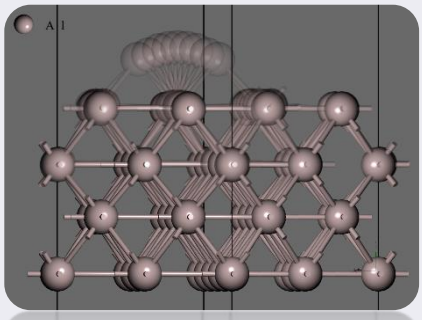
## Analysis of Diffusion Pathways of Al Adatoms Using the NEB Method

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**

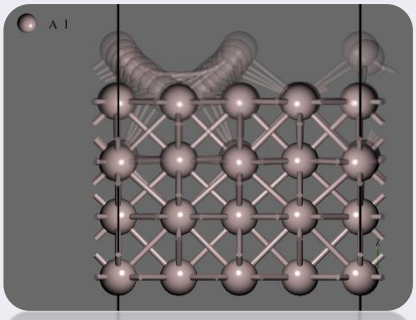
$E_a = 0.46$ eV





**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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Product URL: https://www.nanolabo.advancesoft.jp/en/
Website: https://www.advancesoft.jp/en/