

# APEX Tutorial

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## A. Hands-on APEX Bohrium App

Here we demonstrate how to use APEX Bohrium APP by submitting a computational workflow with the **EAM** pair potential using **LAMMPS** to calculate the **EOS curve** and **elastic properties** of **titanium**.

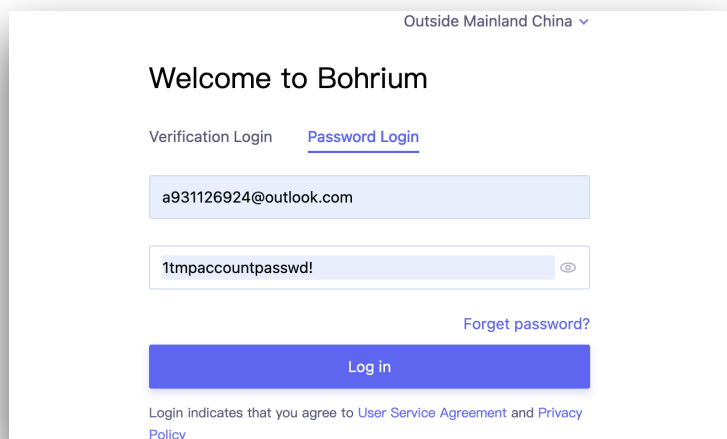
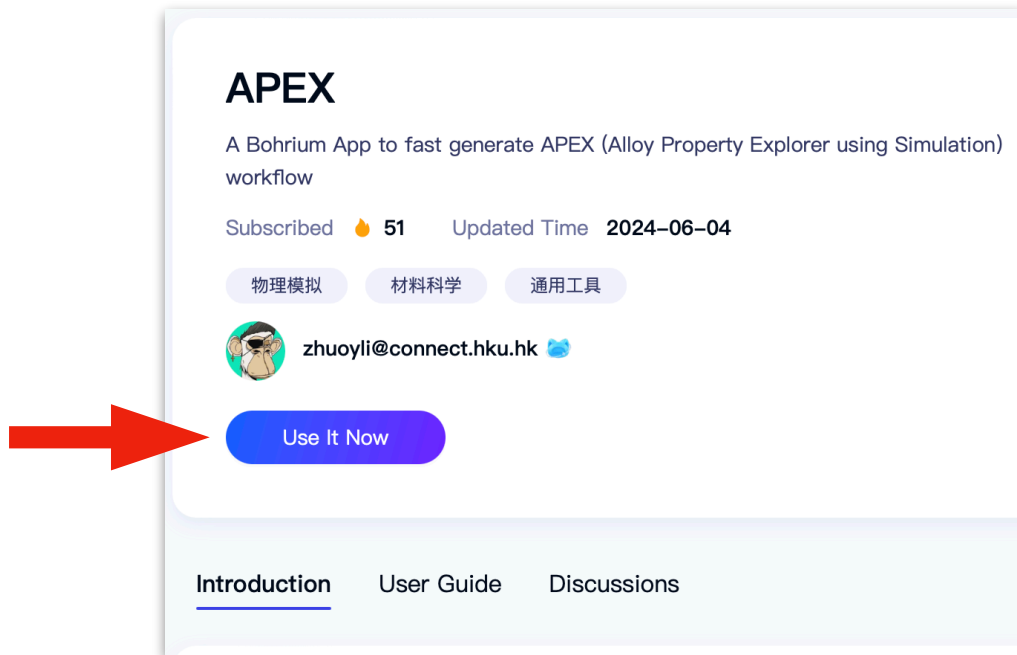
1. Click [here](https://bohrium.dp.tech/apps/apex?tab=readme_link) to enter the main page of **APEX Bohrium App** ([https://bohrium.dp.tech/apps/apex?tab=readme\\_link](https://bohrium.dp.tech/apps/apex?tab=readme_link)), Click the **Use It Now** Button and use following pre-registered temporary **Bohrium** account to login:

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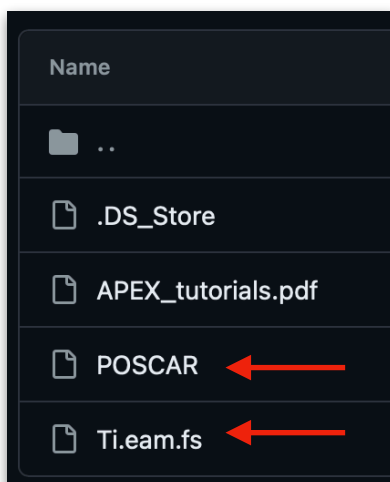
Email: [a931126924@outlook.com](mailto:a931126924@outlook.com)

Password: 1tmpaccountpasswd!

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2. Download two files: the **POSCAR** of HCP Ti ([POSCAR.Ti.hcp](#)) and **EAM potential** file of Ti ([Ti.eam.fs](#)) from [https://github.com/ZLI-afk/static/tree/main/docs/apex\\_Ti\\_test/tutorial](https://github.com/ZLI-afk/static/tree/main/docs/apex_Ti_test/tutorial)



3. Return to the **Form** page, then choose '1-LAMMPS' on the top of the parameter page. Drop the page down, and upload above two files accordingly:

A screenshot of a web form for configuring a LAMMPS simulation. At the top, there are three tabs: '3-ABACUS', '2-VASP', and '1-LAMMPS'. The '1-LAMMPS' tab is selected, indicated by a red arrow. Below the tabs, the text 'Submit MD workflow using LAMMPS' is displayed. The main section is titled 'Job Parameter Configuration'. It contains three sections, each with a title, a help icon, and two buttons: 'Upload from local' and 'Choose from workspace'. The first section is 'Configurations' (marked with a red asterisk), with a red arrow pointing to the 'Upload from local' button. Below the buttons, it says 'Configuration `POSCAR` to be tested (name differently for multiple files)' and shows a file icon labeled 'POSCAR'. The second section is 'Parameter Files', with a red arrow pointing to the 'Upload from local' button. Below the buttons, it says '(Optional) Specify parameter `JSON` files for APEX to override the default settings, (Do not upload if want to do setting manually in the later UI page)' and shows a file icon labeled 'Ti.eam.fs'. The third section is 'Potential Models' (marked with a red asterisk), with a red arrow pointing to the 'Upload from local' button. Below the buttons, it says 'Interatomic potential files required during test' and shows a file icon labeled 'Ti.eam.fs'.

4. Next, drop down the page and check **"Select Elastic"** and **"Select Eos"** in the series of property type boxes. Upon selection, the configuration for computational parameters will expand.



7. Drop to the bottom at “**System Parameter Configuration**” sub–section, Select ‘**APEX Demo**’ in **Project** dropdown, then click the **Submit** button

▼ **System Parameter Configuration**

Job Name

job-apex-9d75831f46204fb882c9240f6f9f3af6

\* Project

APEX Demo

▼

\* Job Machine

CPU /c4\_m8\_cpu ¥ 0.32/hour

recommend

▼

Data saving options

☐ Automatically save the outputs to the project drive(Occupancy rate: 0%)

Data safety options

☒ I agree for developers to collect my task data (input, output, configuration)

Submit

Reset

Estimated Charge = Machine Cost( ¥ 0.32/hour) + License Cost( ¥ 0.00/job)

8. Next, click ‘**Job details**’ for workflow monitoring page

9. On this page, you can monitor the progress of tasks. When the “**Workflow Link**” appears at the right, you can click it to access the Argo workflow monitoring UI page.

✓ Initialization

In this stage, the system is being set up and initialized to prepare for the task. This includes configuring the necessary settings, loading any required data, and initializing any resources that will be used during the task.

✓ PreProcessing

In this stage, the task is being submitted to the system for processing. This involves sending the task request to the server and waiting for a response to confirm that the task has been accepted.

⚙ Running

In this stage, the task is actively being processed by the system. This involves running the necessary algorithms and computations to complete the task, and monitoring the progress to ensure that the task is proceeding as expected.

Job details

Job Report

Submission

Log

Workflow Link

New Line

View All

Running APEX calculation via lammeps

Submitting joint workflow...

Workflow has been submitted (ID: workdir-joint-4x9g2, UID: 2db89d76-1cfe-4ec1-a33f-c837510d73d4)

Workflow link: https://lbg-workflow-mlops.dp.tech/workflows/argo/workdir-joint-4x9g2

Waiting for relaxation result...

Relaxation finished (ID: workdir-joint-4x9g2, UID: 2db89d76-1cfe-4ec1-a33f-c837510d73d4)


Retrieving completed tasks to local...

0%| | 0/1 [00:00<?, ?it/s]

100%| | 1/1 [00:00<00:00, 4.75it/s]

100%| | 1/1 [00:00<00:00, 4.74it/s]

10. You can also click the “**submission**” tab to see detailed running status of all submitted tasks:

 **Running**  
In this stage, the task is actively being processed by the system. This involves running the necessary algorithms and computations to complete the task, and monitoring the progress to ensure that the task is proceeding as expected.

Job details   Job Report   Submission

Job ID	Job Name	Job Status
<a href="#">13886309</a>	<a href="#">job-apex-9d75831f46204fb882c9240f6f9f3af6</a>	Running
<a href="#">13886326</a>	<a href="#">workdir-joint-4x9g2-runlammps-b8nag-9f6wd-8pu01-2733455413</a>	Completed
<a href="#">13886346</a>	<a href="#">workdir-joint-4x9g2-runlammps-b8nag-9f6wd-8pu01-1469084791</a>	Completed
<a href="#">13886347</a>	<a href="#">workdir-joint-4x9g2-runlammps-b8nag-9f6wd-8pu01-768922957</a>	Running ⓘ
<a href="#">13886348</a>	<a href="#">workdir-joint-4x9g2-runlammps-b8nag-9f6wd-8pu01-56817635</a>	Running ⓘ
<a href="#">13886349</a>	<a href="#">workdir-joint-4x9g2-runlammps-b8nag-9f6wd-8pu01-1285747619</a>	Running ⓘ

11. Upon completion of the calculations, all working directories and result files are automatically collected in the /outputs/workdir/ directory, where users can browse and download them into local. The ‘**all\_result.json**’ file can be visualized by `apex report -w all\_result.json` command of any APEX pre-installed GUI computer.

**Workspace** [Go to the project disk](#)

Home / outputs / workdir

Name	Size	LastModTime	Operation
.workflow.log	93.00B	2024-07-19 14:19	
Ti.eam.fs	726.98KB	2024-07-19 14:19	
<u>all_result.json</u>	19.50KB	2024-07-19 14:19	
global_config_tmp.json	1.16KB	2024-07-19 14:19	
parameter_tmp.json	748.00B	2024-07-19 14:19	

## B. Hands-on terminal submission on Bohrium

Please use the following pre-registered temporary Bohrium platform account to access the hands-on demonstration example notebook of APEX

Email: [a931126924@outlook.com](mailto:a931126924@outlook.com)

Password: 1tmpaccountpasswd!

Project\_id: 26924

**Tutorial Notebook link:** <https://nb.bohrium.dp.tech/detail/26383176824>

The screenshot displays the Bohrium platform interface. At the top, the 'English' language dropdown is highlighted with a red box and labeled 'Language switch'. Below the navigation bar, the notebook title 'Hands-on to APEX (v1.2) on Bohrium' is shown. A red arrow points to the 'Connect' button, labeled 'Step 1: Click Connect'. A modal dialog titled 'Select project' is open, showing 'APEX Demo (ID:26924)' selected, with a red box around it and the label 'Step 2: Select "APEX Demo"'. The modal also shows 'System-created default p... (ID:26925)' as an option. The background content includes a 'Getting Started Guide' section with instructions on how to execute the notebook directly on the Bohrium platform.