

# 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**.

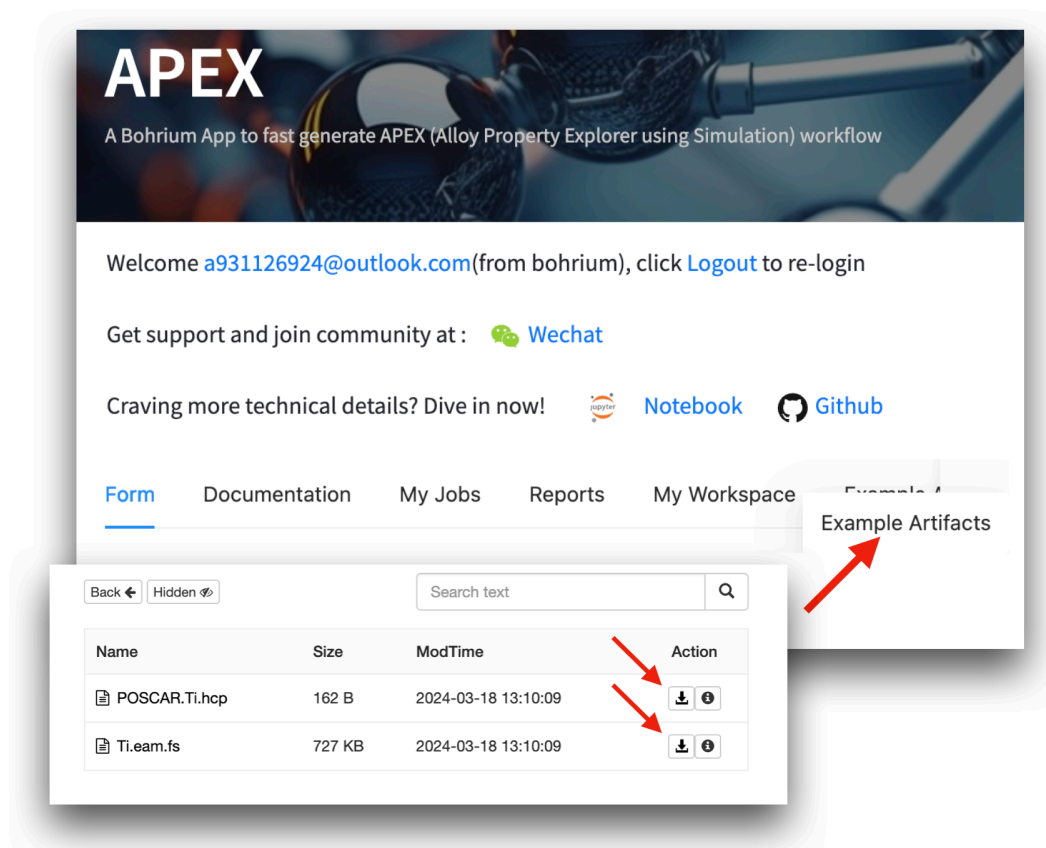
1. Click [here](https://app.bohrium.dp.tech/apex/) to enter the main page of **APEX Bohrium App** (<https://app.bohrium.dp.tech/apex/>), and use following pre-registered temporary Bohrium account to login:

\_\_\_\_\_  
Email: \_\_\_\_\_

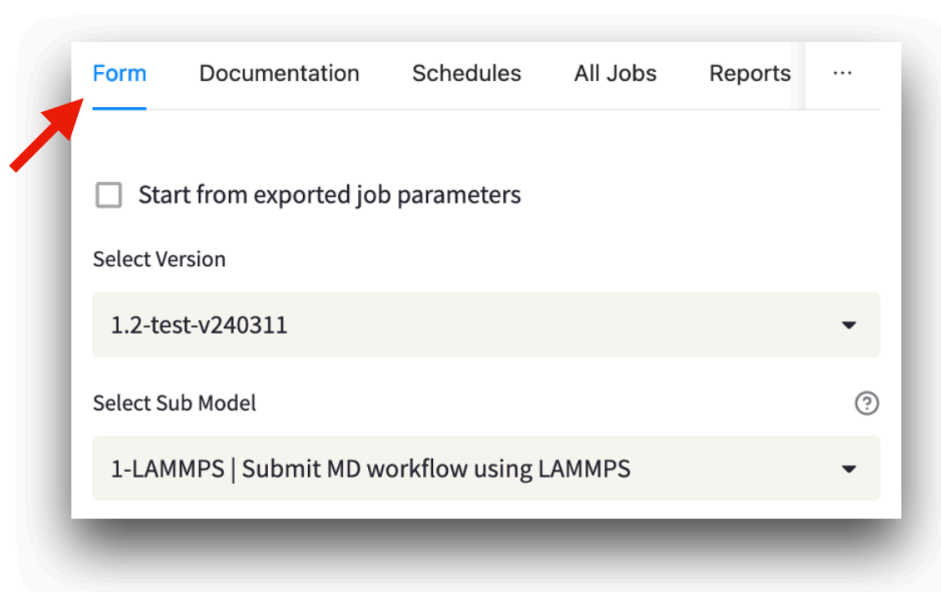
Password: \_\_\_\_\_



- At the top right, click **Example Artifacts** and download two files: the **POSCAR** of HCP Ti ([POSCAR.Ti.hcp](#)) and **EAM potential** file of Ti ([Ti.eam.fs](#))



- Return to the **Form** page, then select the relevant version 1.2 from the **Select Version** dropdown menu in the Form page, and then choose '**1-LAMMPS**' in the **Select Sub Model** section below:



4. Drop the page down, and upload above two files accordingly:

The screenshot shows a web interface for uploading files. It has two main sections: 'Configurations' and 'Potential Models'. Each section has a header with a description, a sub-header, and two tabs: 'Upload from local' (selected) and 'Choose from workspace'. Below the tabs is a file upload area with a 'Drag and drop files here' instruction, a 'Limit 500MB per file' note, and a 'Browse files' button. A red arrow points from the text 'POSCAR.Ti.hcp' to the 'Browse files' button. Below the upload area, a file 'POSCAR.Ti.hcp' (162.0B) is listed with a close button. A dropdown menu shows 'Fail to open a file selection dialog?'. The 'Potential Models' section follows the same layout, with a red arrow pointing from 'Ti.eam.fs' to its 'Browse files' button, and a file 'Ti.eam.fs' (0.7MB) listed below.

Configurations (Configuration `POSCAR` to be tested (name differently for multiple files))

Upload from local Choose from workspace

POSCAR.Ti.hcp

Drag and drop files here  
Limit 500MB per file

Browse files

POSCAR.Ti.hcp 162.0B

Fail to open a file selection dialog?

Potential Models (Interatomic potential files required during test)

Upload from local Choose from workspace

Ti.eam.fs

Drag and drop files here  
Limit 500MB per file

Browse files

Ti.eam.fs 0.7MB

5. Drop to the page bottom and click **Next** button to parameter setting page, and set global computing configuration

The screenshot shows a parameter setting page for LAMMPS simulation. It has several fields with descriptions and a question mark icon. The fields are: 'Lammps Image Name' (registry.dp.tech/dptech/prod-11045/deepmdkit-phonolammps:2.1.1), 'Lammps Run Command' (lmp -in in.lammps), 'Apex Image Name' (registry.dp.tech/dptech/prod-11045/apex-dependency:1.2.0), 'Scass Type' (c8\_m31\_1 \* NVIDIA T4), 'Group Size' (2), and 'Pool Size' (1). Each field has a minus and plus button for adjustment.

Lammps Image Name (LAMMPS image address for MD simulation) ?

registry.dp.tech/dptech/prod-11045/deepmdkit-phonolammps:2.1.1

Lammps Run Command (LAMMPS run command (lmp instruction file name should be `in.lammps`)) ?

lmp -in in.lammps

Apex Image Name (Image address including dependencies for APEX to run) ?

registry.dp.tech/dptech/prod-11045/apex-dependency:1.2.0

Scass Type (Bohrium machine node type for MD simulation) ?

c8\_m31\_1 \* NVIDIA T4

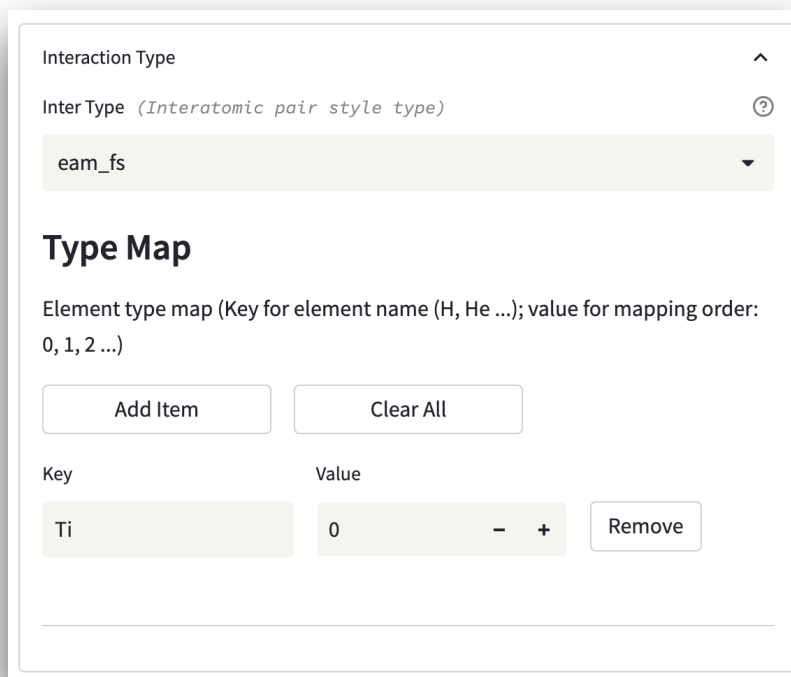
Group Size (Number of tasks per parallel run group) ?

2 - +

Pool Size (For multi tasks per parallel group, the pool size of multiprocessing pool to handle each task (1 for serial, -1 for infinity)) ?

1 - +

6. Next, set up atomic interaction details. Select "**eam\_fs**" from the **Inter Type** dropdown, and add one key-value pair {Ti: 0} in the **Type Map** area.



Interaction Type ^

Inter Type *(Interatomic pair style type)* ?

eam\_fs ▼

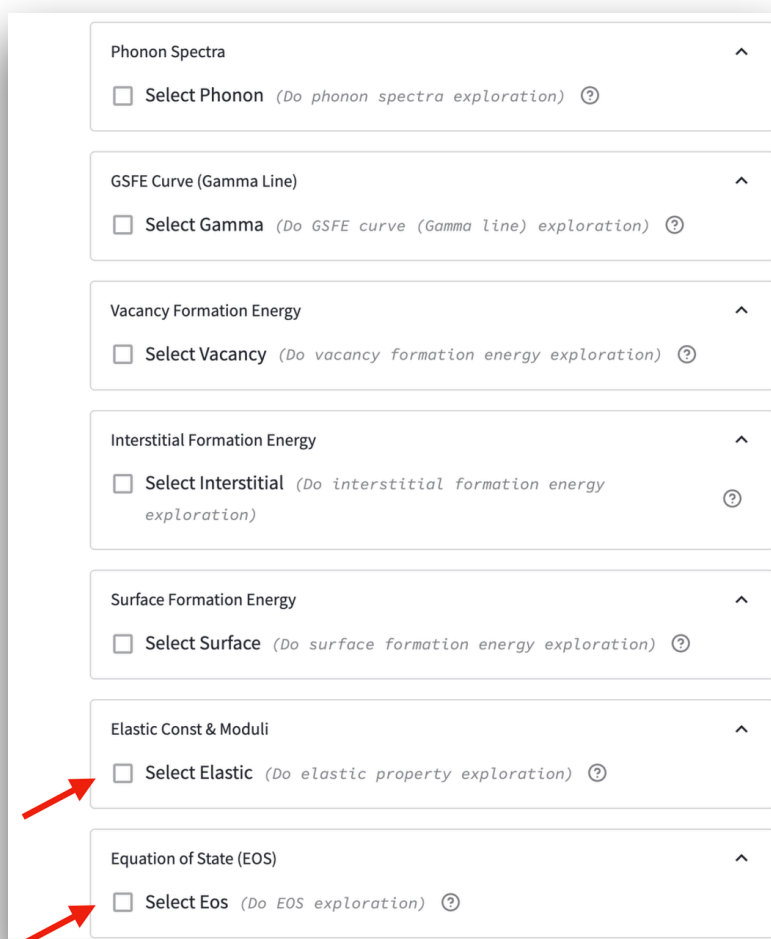
### Type Map

Element type map (Key for element name (H, He ...); value for mapping order: 0, 1, 2 ...)

Add Item Clear All

Key	Value	
Ti	0	- + Remove

7. Next, check "**Select Elastic**" and "**Select Eos**" in the series of property type boxes. Upon selection, the configuration for computational parameters will expand. Then, drop to the page bottom and click **Next** button



Phonon Spectra ^

☐ Select Phonon *(Do phonon spectra exploration)* ?

GSFE Curve (Gamma Line) ^

☐ Select Gamma *(Do GSFE curve (Gamma line) exploration)* ?

Vacancy Formation Energy ^

☐ Select Vacancy *(Do vacancy formation energy exploration)* ?

Interstitial Formation Energy ^

☐ Select Interstitial *(Do interstitial formation energy exploration)* ?

Surface Formation Energy ^

☐ Select Surface *(Do surface formation energy exploration)* ?

Elastic Const & Moduli ^

☐ Select Elastic *(Do elastic property exploration)* ?

Equation of State (EOS) ^

☐ Select Eos *(Do EOS exploration)* ?

8. Click **Next** button again to the final submission page.
9. Drop to the bottom, Select '**APEX Demo**' in **Bohrium Project** dropdown, then check the 'I agree to the term and conditions' before clicking final **Submit** button

Job Prefix

Bohrium Project

APEX Demo(ID=26924, Collaborative Project)

You have one or more Experience Cards available in your owned project(s). Please note that if you choose to use your owned project for payment, the Experience Card(s) will be prioritized for billing.

💡 Top up to maintain optimal performance!

Job Description (Optional)

Submit MD workflow using LAMMPS

SUBMIT TO PURCHASE 🛒

Item	Price(¥)
One-time License	0
Resources utilized by the job for computing purposes	Δ(Pay As You Go)

☒ I agree to the terms and conditions

Submit

Prev

10. Next, click '**Job details**' for workflow monitoring page

✓

## Job Created Successfully!

job name: job-apex-1.2-test-v240311-896d90. The job running takes a few minutes, please wait.

Job details Create a new job Back edit

11. On this page, you can monitor the progress of tasks. When the **"Workflow"** tab appears at the top, you can click it to access the workflow monitoring page.

**Job : job-apex-1.2-test-v240311-e17261 (running)**

created at 2024-03-13T15:14:04.237268 by zhuoyli@connect.hku.hk, v

☐ Job Owner Access Exclusive  
☒ Only collaborators of the job can access via link  
☐ Anyone with the link can view

[Main](#) [Metrics](#) [Workflow](#) [Export](#)

**Force Stop**

Job has been submitted, details can be found here <https://bohrium.dp.tech/jobs>

- Bohrium job id: 11498554, group id: 11766527

Estimated job cost: ¥0.0 in utility(Pay As You Go), ¥ 0 for the license.

Description

Submit MD workflow using LAMMPS

**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

12. 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.

**Success**  
In this stage, the task is success and you can check results.

Job Workspace

[/ outputs / workdir /](#)

[Back](#) [Hidden](#)  [Q](#)

Name	Size	ModTime	Action
returns	~1.8 MB	2024-03-13 15:33:32	<a href="#">Zip</a> <a href="#">Download</a> <a href="#">Info</a>
parameter_tmp.json	748 B	2024-03-13 15:33:32	<a href="#">Download</a> <a href="#">Info</a>
global_config_tmp.json	1 KB	2024-03-13 15:33:32	<a href="#">Download</a> <a href="#">Info</a>
all_result.json	19 KB	2024-03-13 15:33:32	<a href="#">Download</a> <a href="#">Info</a>
Ti.eam.fs	727 KB	2024-03-13 15:33:32	<a href="#">Download</a> <a href="#">Info</a>

## 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: \_\_\_\_\_

Password: \_\_\_\_\_

Project\_id: \_\_\_\_\_

Tutorial Notebook link: \_\_\_\_\_

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 visible. 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 and 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.