APEX Tutorial

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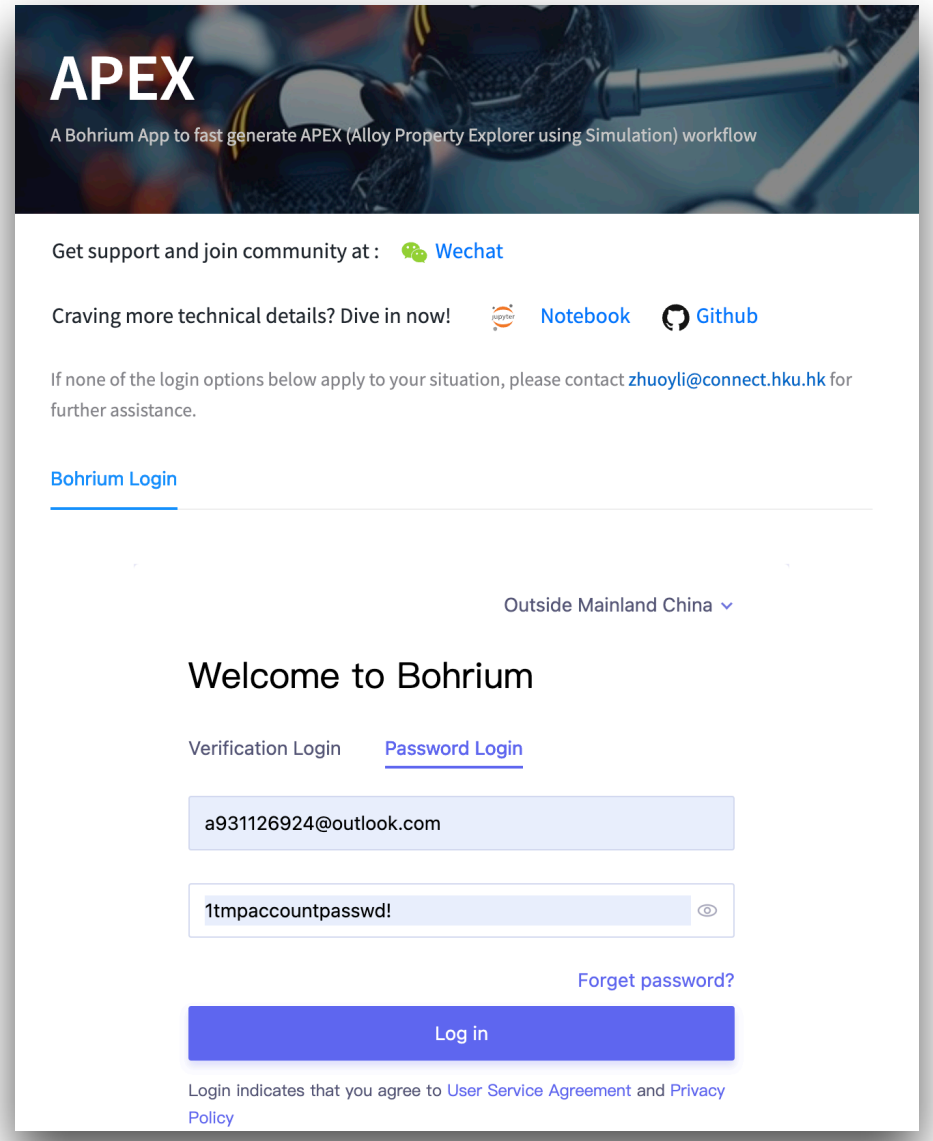
A. Hands-on APEX Bohrium App

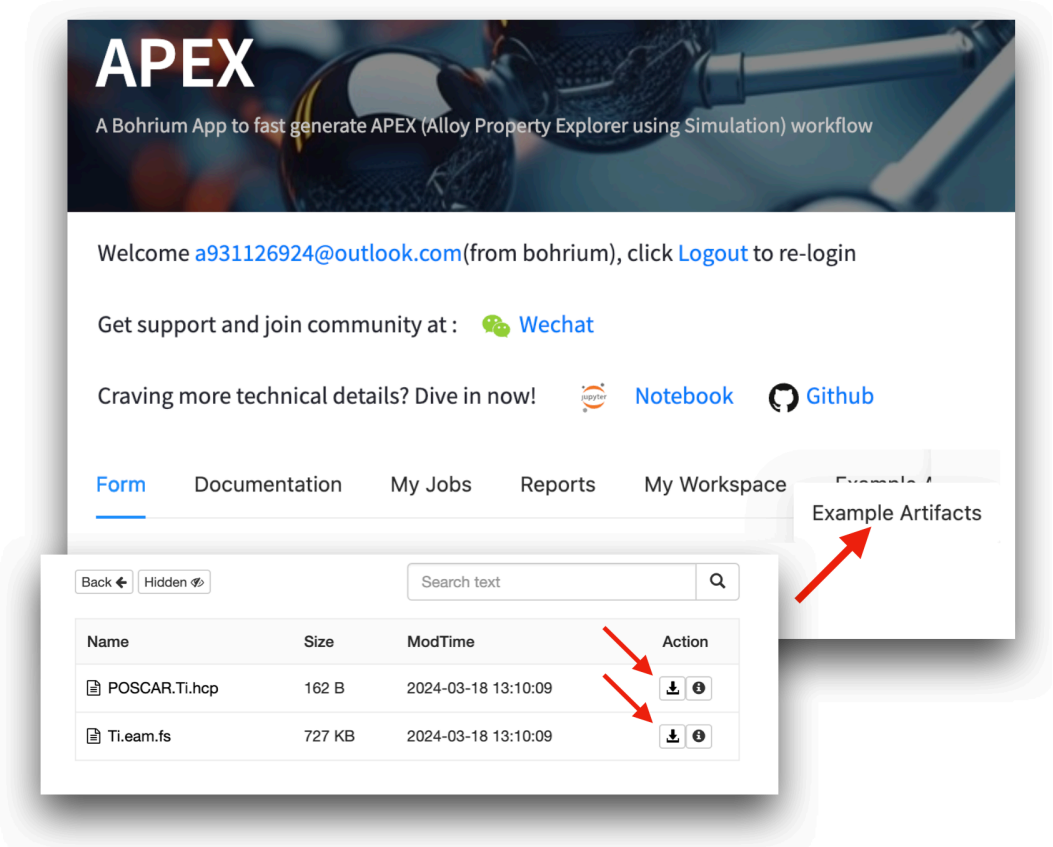
Here we demonstrate how to use APEX Bohrium APP by submitting a computational workflow with the **EAM** pair potential using **LAMMPS** to calculate the **EOS curve** and **elastic properties** of **titanium**.

1. Click **here** 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:

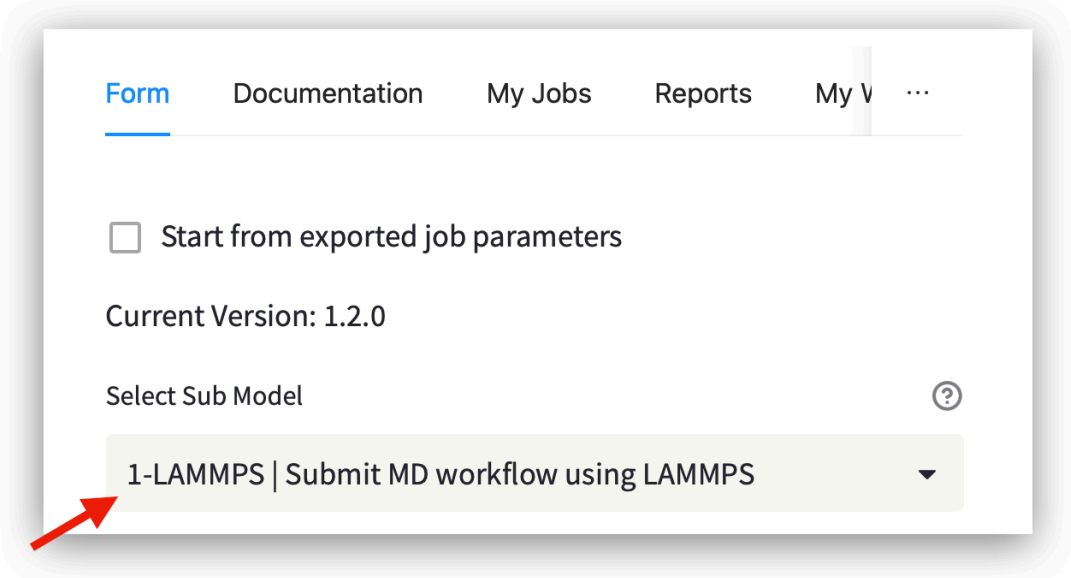
   Email: a931126924@outlook.com
   Password: 1tmpaccountpasswd!



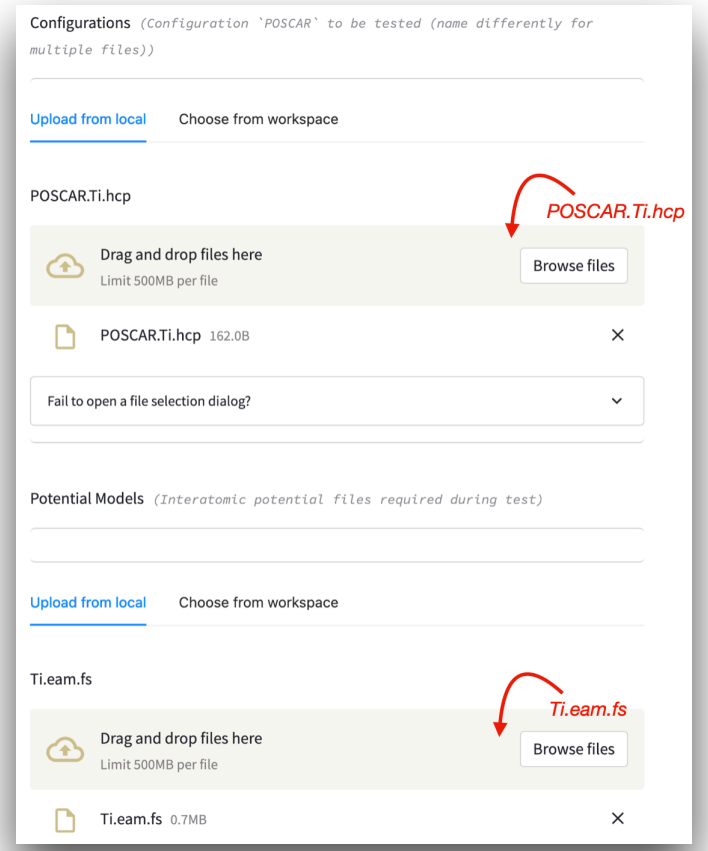
2. At the top right, click **Example Artifacts** and download two files: the **POSCAR** of HCP Ti (POSCAR.Ti.hcp) and **EAM potential** file of Ti (Ti.eam.fs)



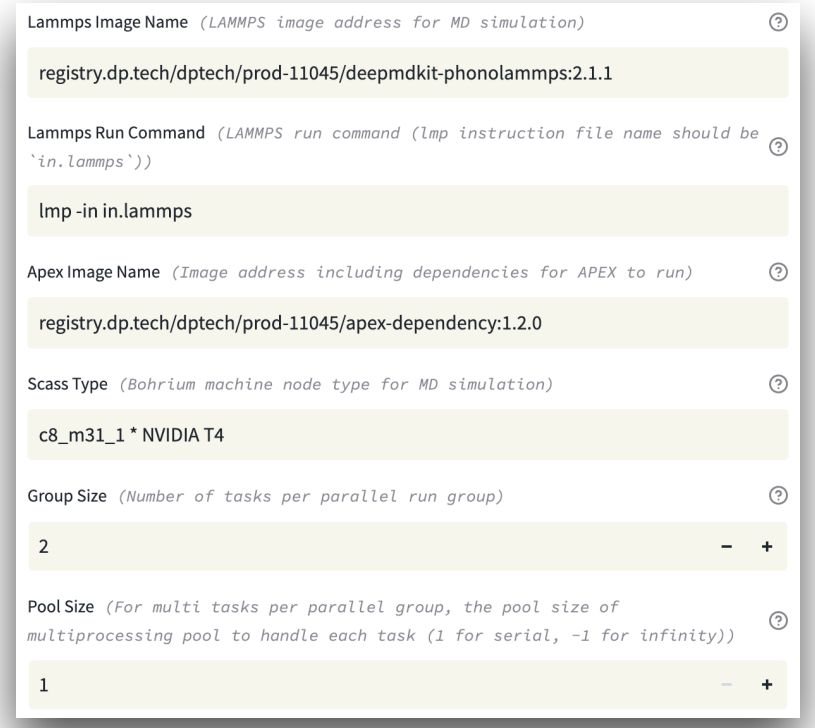
3. Return to the **Form** page, then choose **'1–LAMMPS'** in the **Select Sub Model** section below:



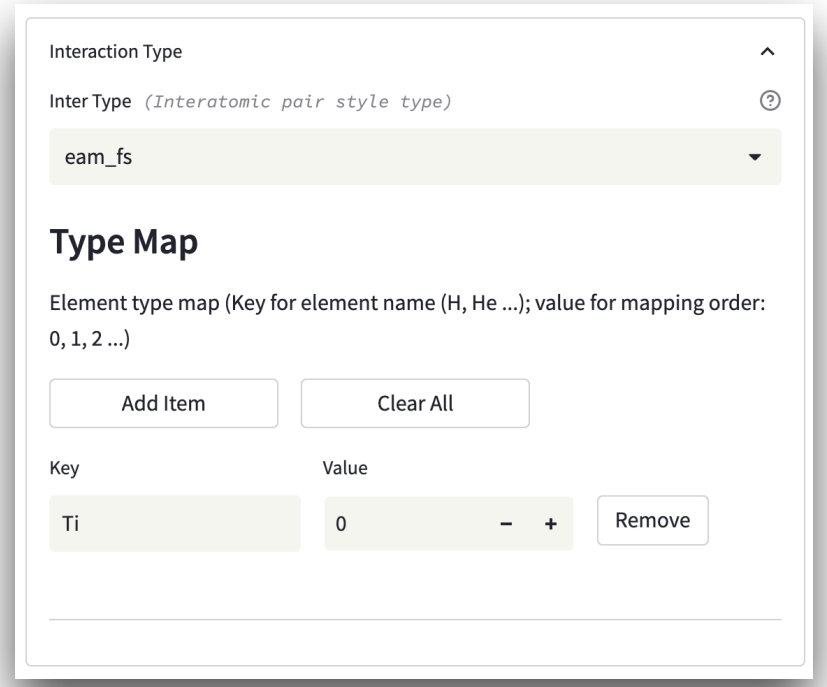
4. Drop the page down, and upload above two files accordingly:



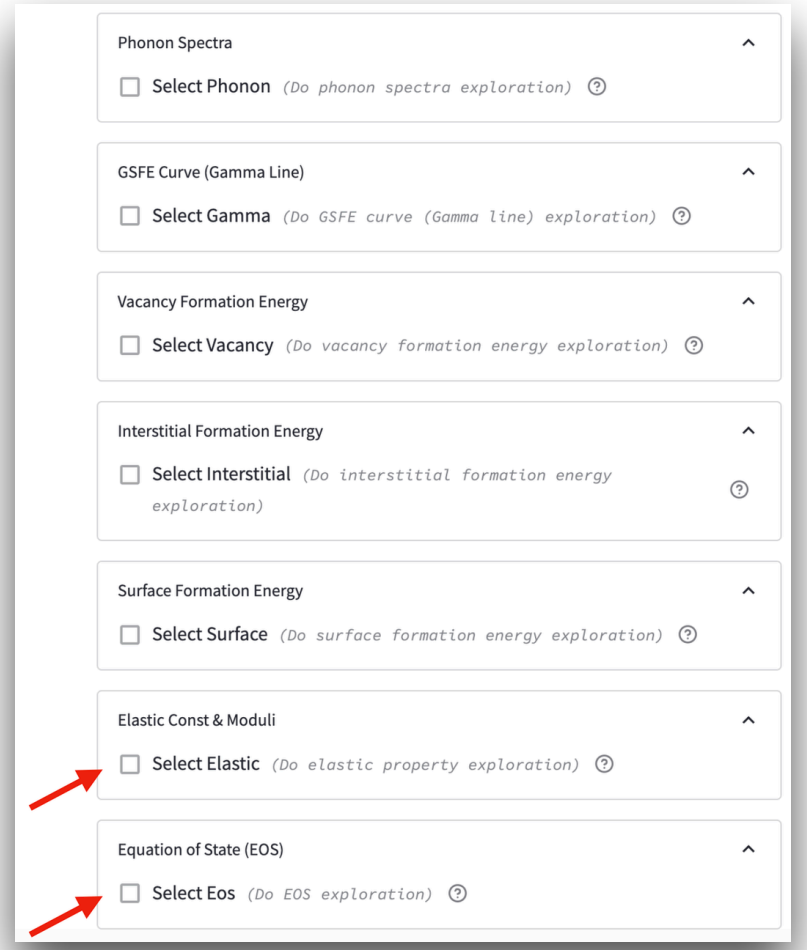
5. Drop to the page bottom and click **Next** button to parameter setting page, and set global computing configuration



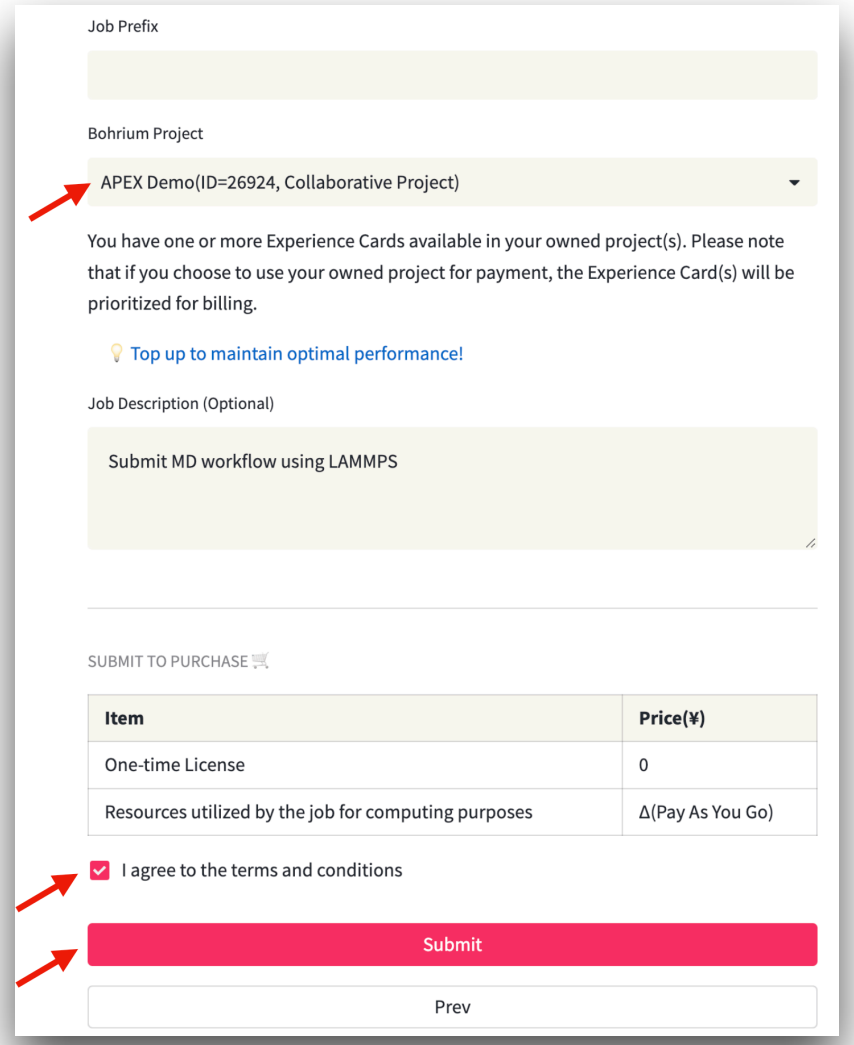
6. Next, set up atomic interaction details. Select **"eam_fs"** from the **Inter Type** dropdown, and add one key–value pair **{Ti: 0}** in the **Type Map** area.



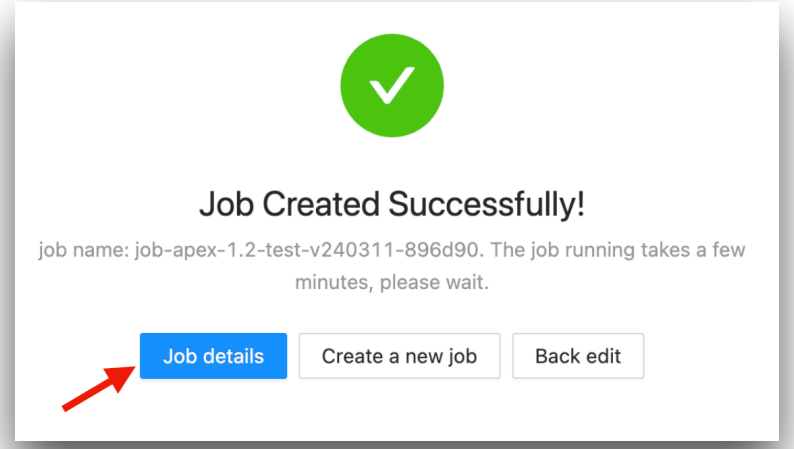
7. Next, check **"Select Elastic"** and **"Select Eos"** in the series of property type boxes. Upon selection, the configuration for computational parameters will expand. Then, drop to the page bottom and click **Next** button



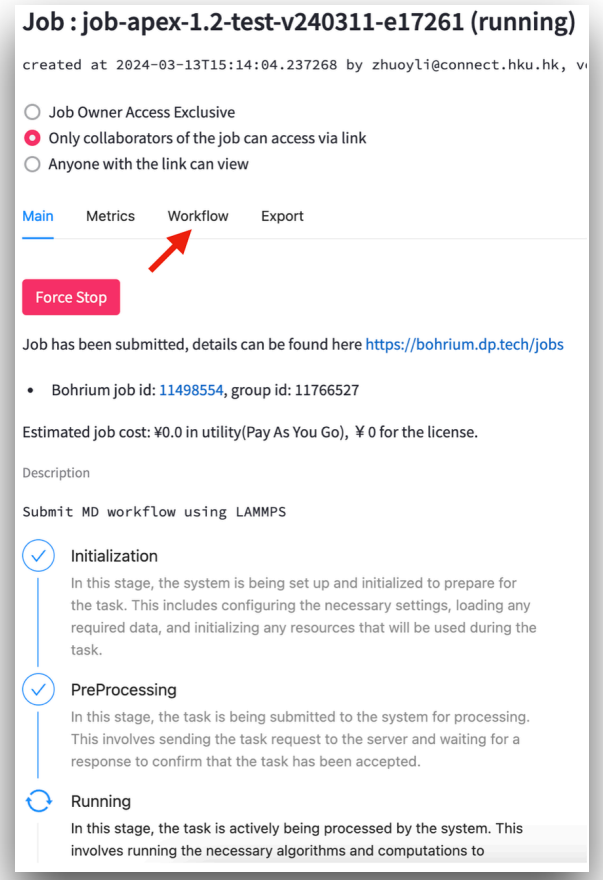
8. Click **Next** button again to the final submission page.
9. Drop to the bottom, Select **'APEX Demo'** in **Bohrium Project** dropdown, then check the 'I agree to the term and conditions' before clicking final **Submit** button



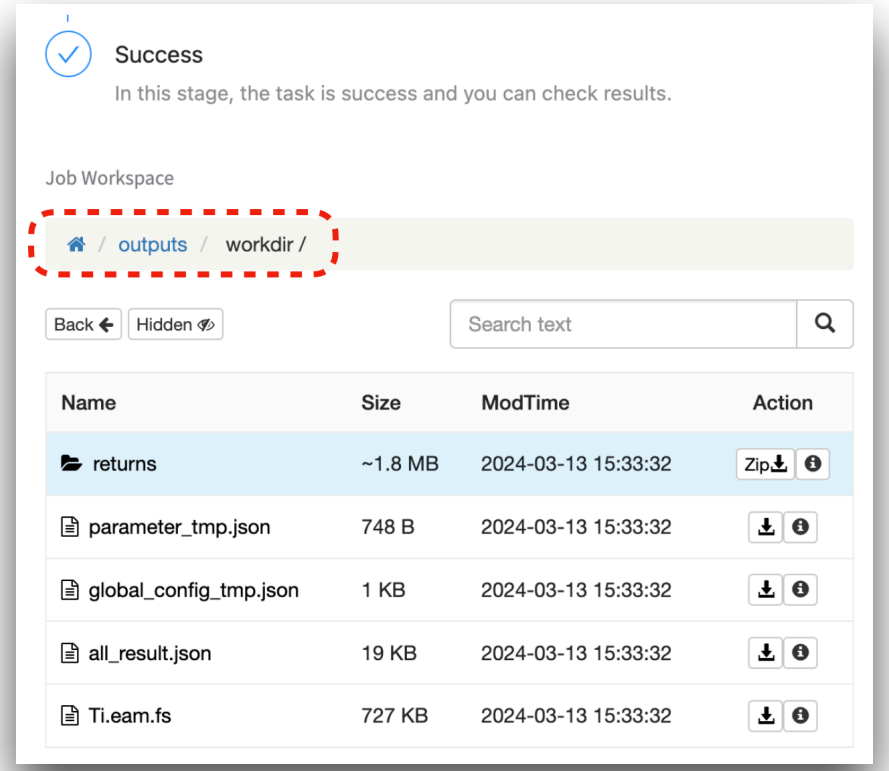
10. Next, click **'Job details'** for workflow monitoring page



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 (Keep refreshing the page to see the newest workflow status).



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.



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
Password: 1tmpaccountpasswd!
Project_id: 26924

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