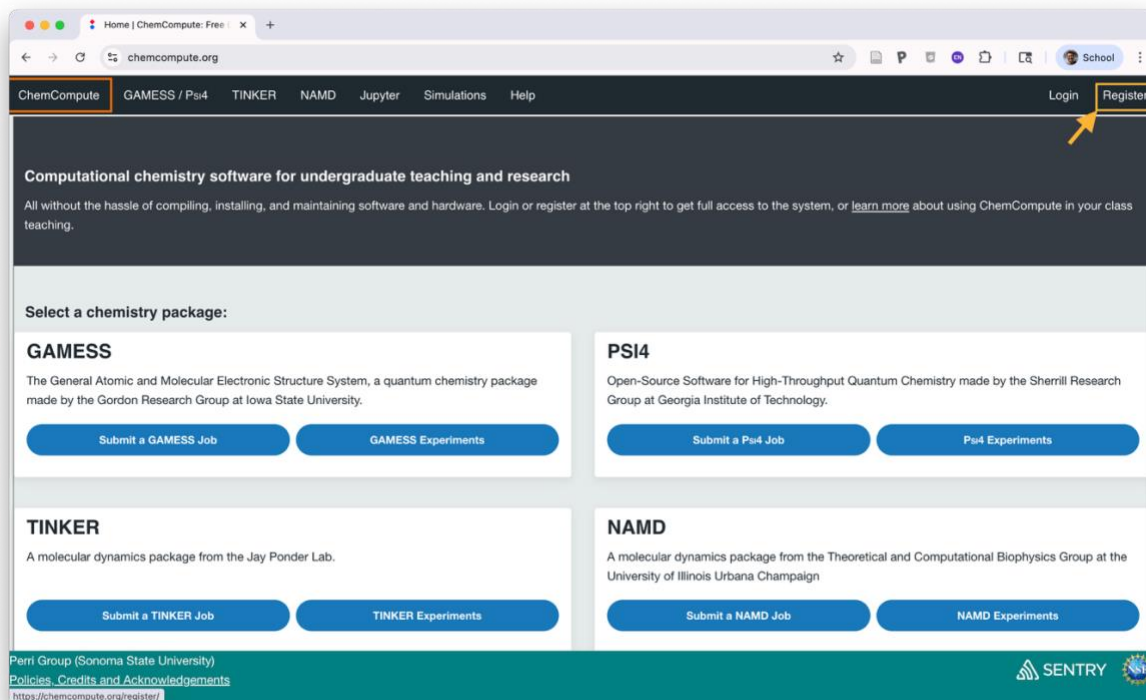
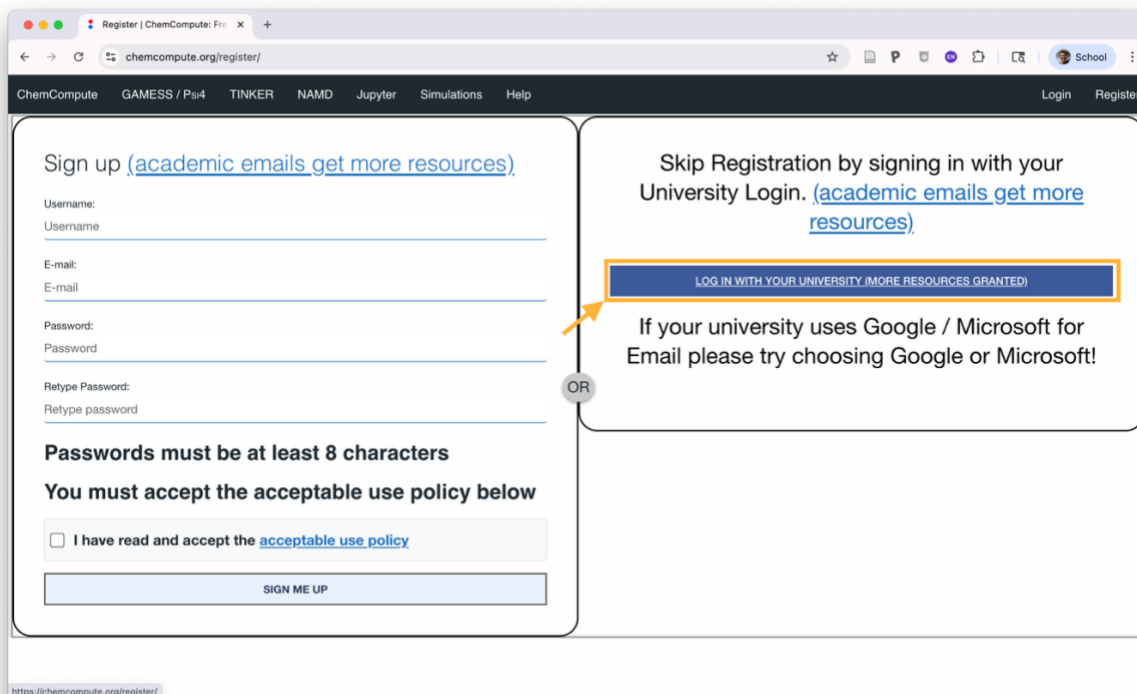


Document 1: Getting Started

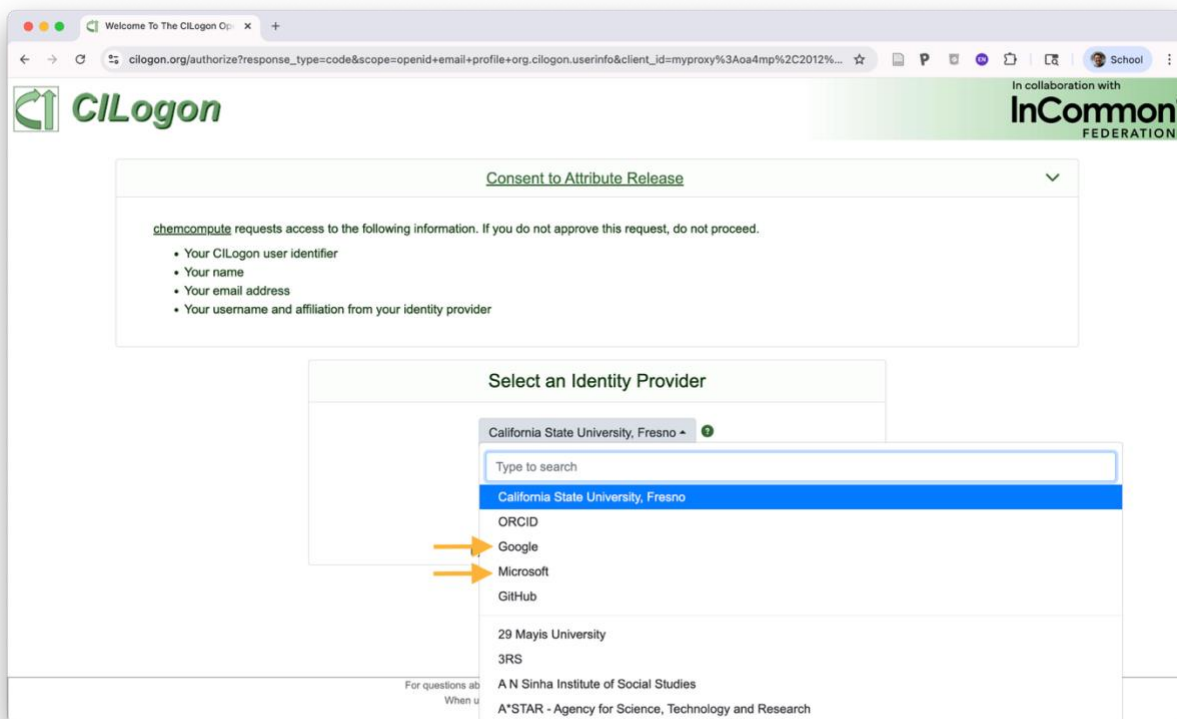
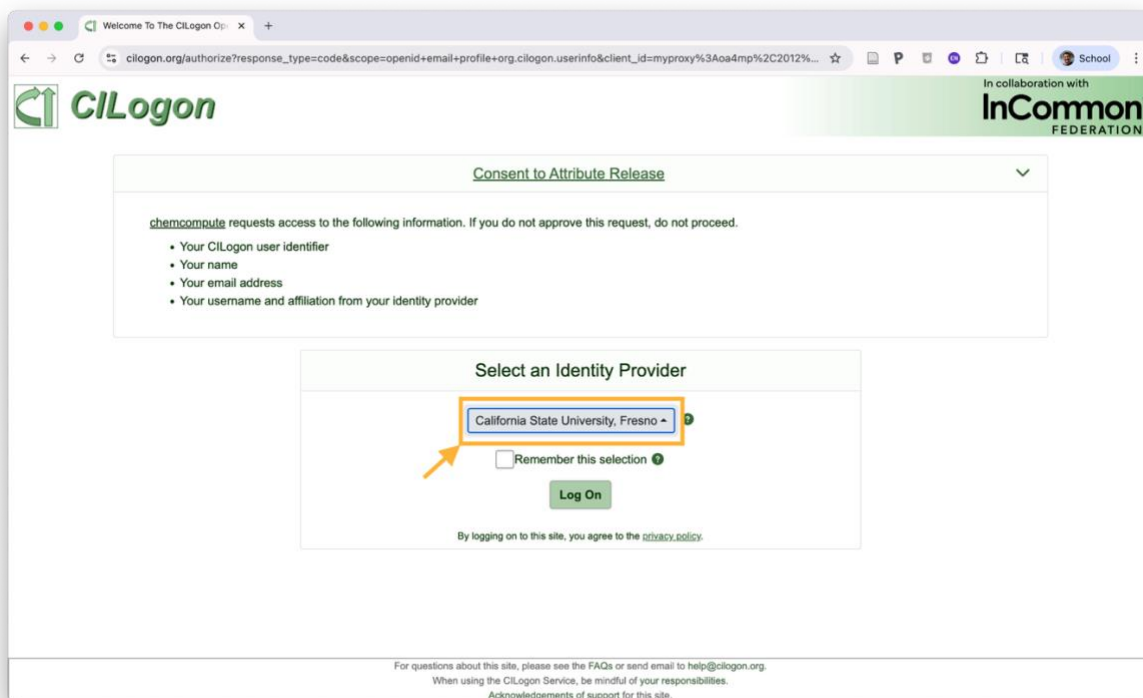
1. In your web browser, look up ChemCompute or enter this link into your address bar <https://chemcompute.org/>.
2. If you do not have an existing account with ChemCompute, you will need to register for one now (this is free).



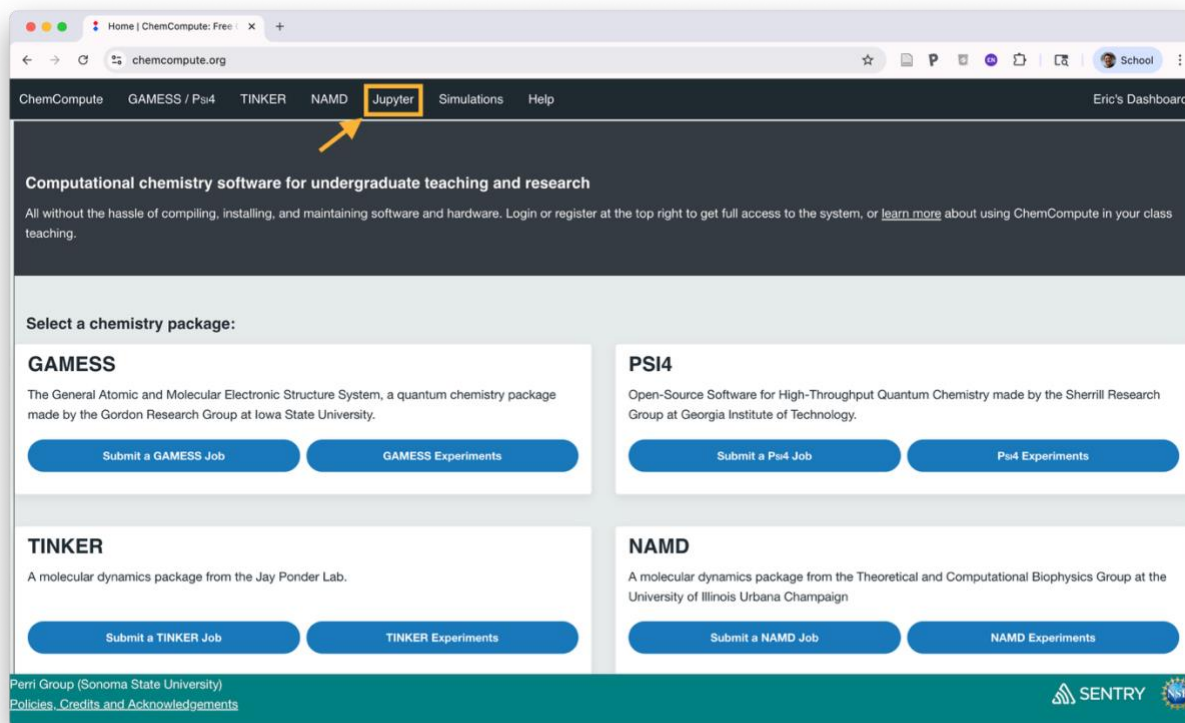
3. Login with your University Login.



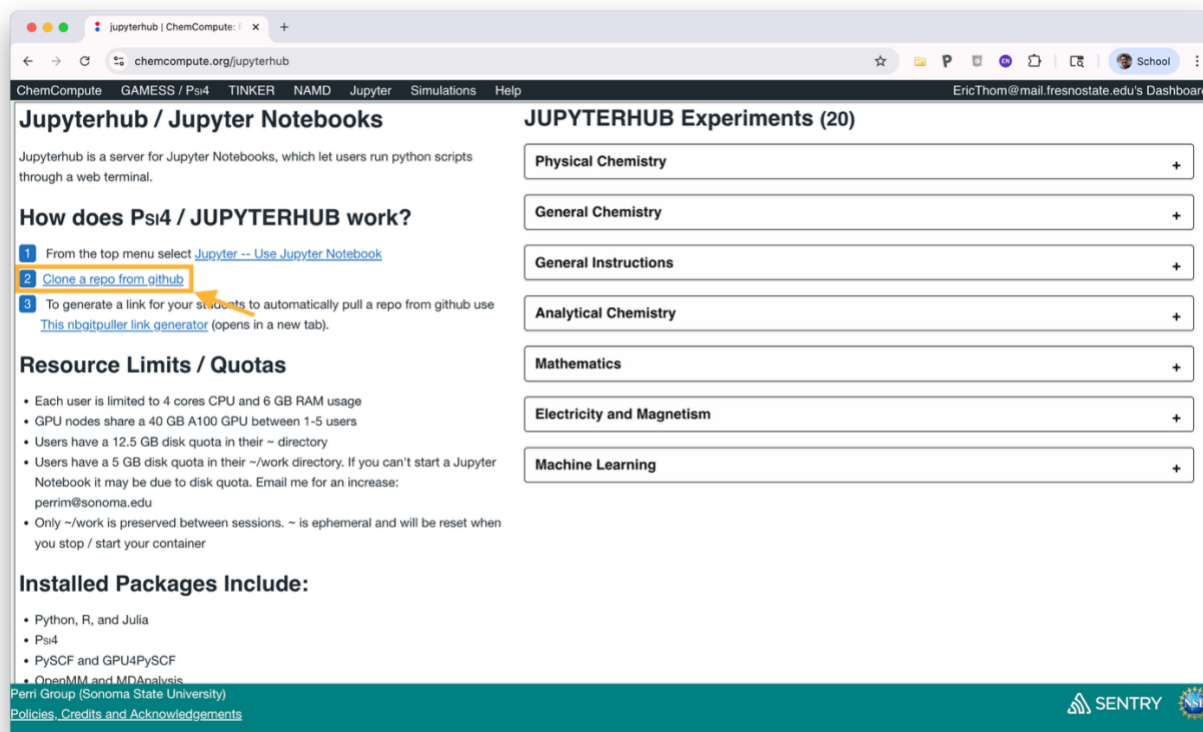
4. Select your Identity Provider from the dropdown menu. If your school is not listed, select a third-party identity provider based on your school account. If your student email uses Google, select “Google”. If your student email uses Outlook, select “Microsoft”.



5. Select Jupyter (Dropdown menu when hovering is not relevant).



6. Select “clone a repo from github”.



7. Paste the URL <https://github.com/Cheman27/Hybridization-Activity.git> into the designated portion, then select “Clone Repo” button.

Launch a Jupyter Notebook

chemcompute.org/jupyterhub/git

ChemCompute GAMESS / Psi4 TINKER NAMD Jupyter Simulations Help Show Instructions EricThorn@mail.fresnostate.edu's Dashboard

Follow these steps clone a repo from github:

1. Login to ChemCompute with an academic account [Logged In](#) Verified Academic Account
2. Start a notebook instance then return to this tab [Start Notebook](#)
3. Enter the URL of the repo you want to clone
4. Click the "Clone Repo" button

URL:

Optional: enter branch (if not master or main)

Optional: choose between Jupyter Notebook (default) or Jupyter Lab

[Clone Repo](#)

To generate a link for your students to automatically pull a repo from github use [This nbgitpuller link generator](#)

8. Once redirected, ensure “Select a language” option is set to “Python” and the “Select how to provide the image” option is set to “Select a Premade image (default)”, and lastly, you will need to change “Select between Images” by clicking on the dropdown menu.

Launch a Jupyter Notebook

JupyterHub

chemcompute.org/jupyterhub_internal/hub/spawn/788bea8685dfd45965e70039892a4b41?next=%2Fjupyterhub_internal%2Fuser%2F788... Logout

jupyterhub Home Token 788bea8685dfd45965e70039892a4b41 Logout

Server Options

ChemCompute has two options for your notebook. It can run on a regular node (CPU node) or a GPU node. A GPU node has access to a graphics card, which can be used to make certain calculations run faster.

If you know that you need access to a GPU, choose GPU node and image ≥ 1.10 . If you're not sure, choose CPU node.

GPU nodes take a few minutes to start up. CPU nodes should be immediately available.

Notebooks on GPU nodes will be shut off if the GPU is idle for an hour

Select an instance for your notebook

Select between Jupyter Notebook and Jupyter Lab

Select a language:

☒ Python ☐ R ☐ Julia

Select how to provide the image:

☒ Select a Premade Image (default)

☐ Use a custom repository. These must be [approved](#)

Select between Images

Python 3.12.11

[Start](#)

9. From the dropdown menu select “1.16 (Nov25) – psi4 v1.10rebuilt with angular momentum 6. Update python to 3.12.11”.

Launch a Jupyter Notebook | JupyterHub

chemcompute.org/jupyterhub_internal/hub/spawn/788bea8685dfd45965e70039892a4b41?next=%2Fjupyterhub_internal%2Fuser%2F78... | School

jupyterhub Home Token 788bea8685dfd45965e70039892a4b41 Logout

Server Options

ChemCompute has two options for your notebook. It can run on a regular node (CPU node) or a GPU node. A GPU node has access to a graphics card, which can be used to make certain calculations run faster.

If you know that you need access to a GPU, choose GPU node and image >= 1.10. If you're not sure, choose CPU node.

GPU nodes take a few minutes to start up. CPU nodes should be immediately available.

Notebooks on GPU nodes will be shut off if the GPU is idle for an hour

Select an instance for your notebook: CPU node (default)

Select between Jupyter Notebook and Jupyter Lab: Jupyter Notebook (default)

Select a language:
☒ Python ☐ R ☐ Julia

Select how to provide the image:
☒ Select a Premade Image (default)
☐ Use a custom repository. These must be [preapproved](#)

Select between Images

- 2.1 (Jan 26) -- Upgrade to Notebook v7: Major Accessibility Improvements
- ✓ 1.16 (Nov 25) -- psi4 v1.10 rebuilt with angular momentum 6. Update python to 3.12.11**
- 1.15 (Oct 25) -- Added jupyter_myst
- 1.14 (Apr 25) -- Added sweetviz, pandastools.
- 1.13 (Feb 25) -- Install pdb2pqr, meeko, proliif, pdbfixer, adme-py, smileite. Update pandas=2.2.3, openmm=8.2.0
- 1.12 (Feb 25) -- added pubchempy, langchain, openai
- 1.11 (Aug 24) -- Update Psi4 to 1.9.1, add gpu4pyscf
- 1.10 (Jul 24) -- GPU drivers updated
- 1.9 (Jul 24) -- added jupyterlab-git, vina, rcsbsearchapi, WebIO

10. Now click Start.

Launch a Jupyter Notebook | JupyterHub

chemcompute.org/jupyterhub_internal/hub/spawn/788bea8685dfd45965e70039892a4b41?next=%2Fjupyterhub_internal%2Fuser%2F78... | School

jupyterhub Home Token 788bea8685dfd45965e70039892a4b41 Logout

Server Options

ChemCompute has two options for your notebook. It can run on a regular node (CPU node) or a GPU node. A GPU node has access to a graphics card, which can be used to make certain calculations run faster.

If you know that you need access to a GPU, choose GPU node and image >= 1.10. If you're not sure, choose CPU node.

GPU nodes take a few minutes to start up. CPU nodes should be immediately available.

Notebooks on GPU nodes will be shut off if the GPU is idle for an hour

Select an instance for your notebook: CPU node (default)

Select between Jupyter Notebook and Jupyter Lab: Jupyter Notebook (default)

Select a language:
☒ Python ☐ R ☐ Julia

Select how to provide the image:
☒ Select a Premade Image (default)
☐ Use a custom repository. These must be [preapproved](#)

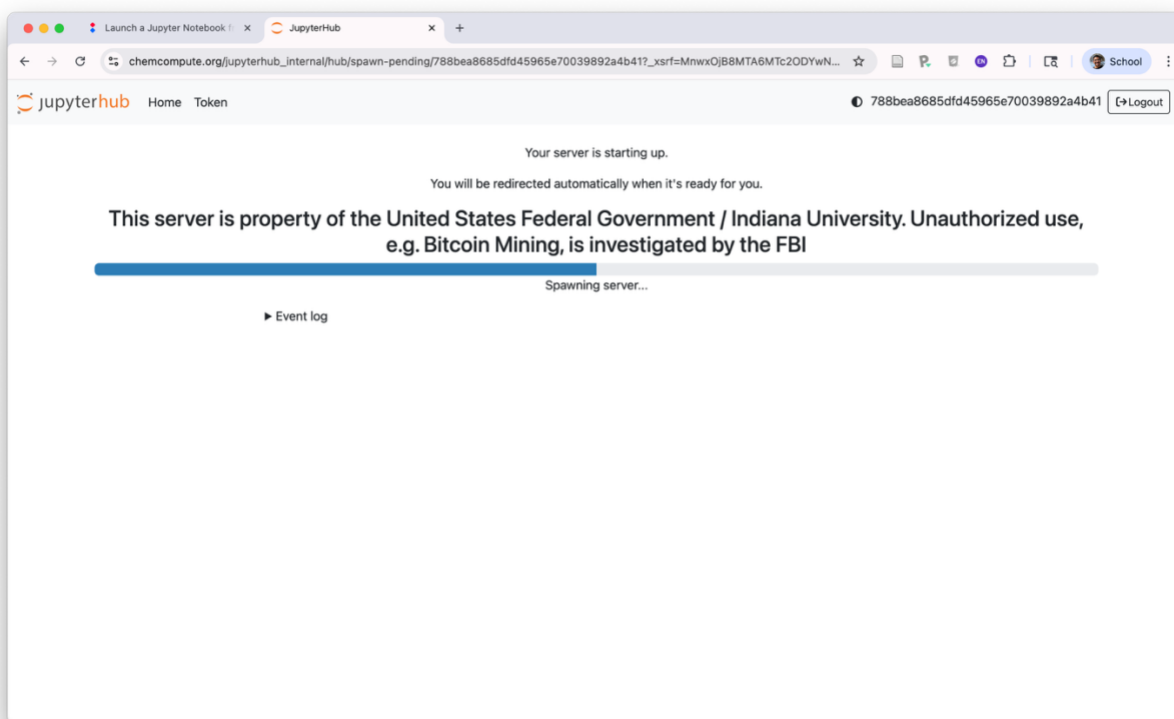
Select between Images

1.16 (Nov 25) -- psi4 v1.10 rebuilt with angular momentum 6. Update python to 3.12.11

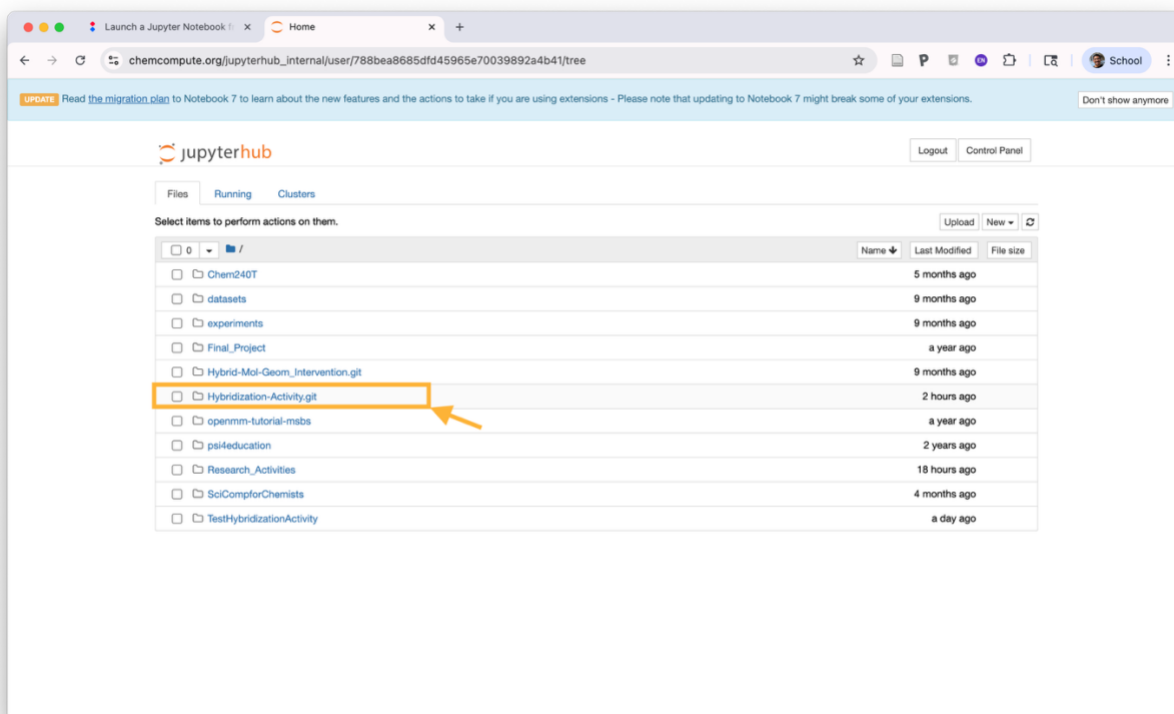
Python 3.12.11

Start

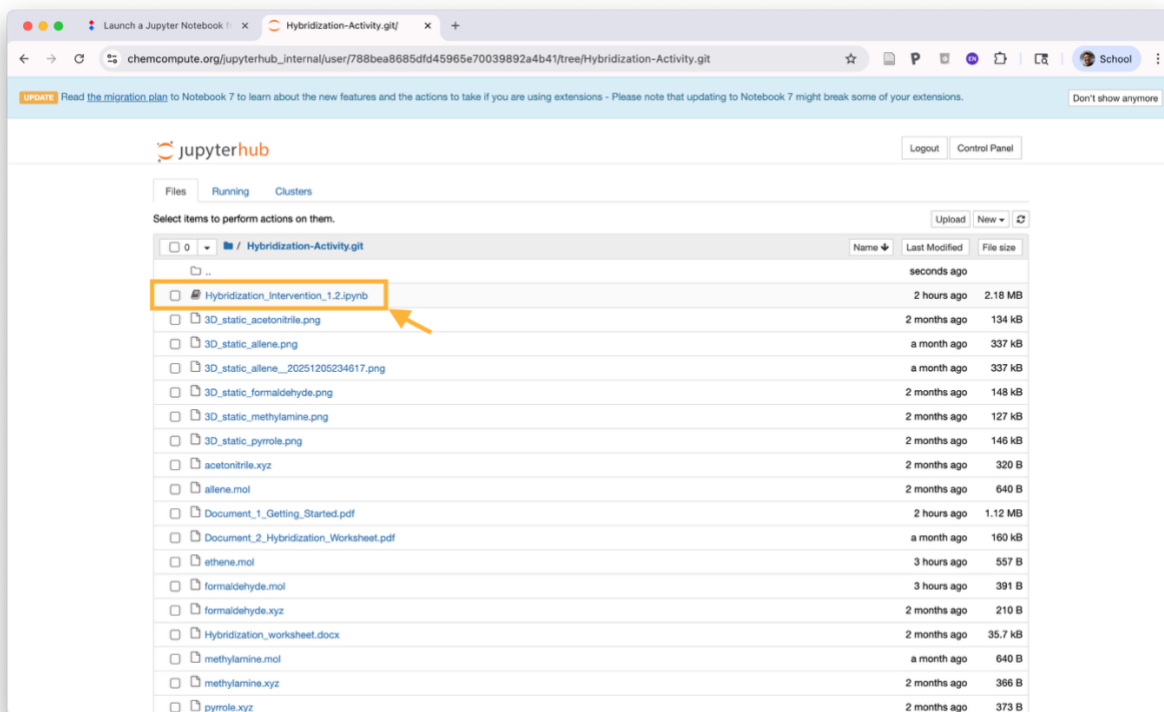
11. You will be redirected to a new tab. This may take a while if multiple students are setting up at the same time on the same server.



12. Once loading is complete, press Hybridization-Activity.git. Do not worry if your screen does not show as many folders as the image below. It is only important that you have the Hybridization-Activity.git folder.



13. Select “Hybridization_Intervention_1.2.ipynb”. You will be redirected to one more tab.



14. Now that you can access your Jupyter notebook, **proceed to Document 2: Hybridization Worksheet.**

