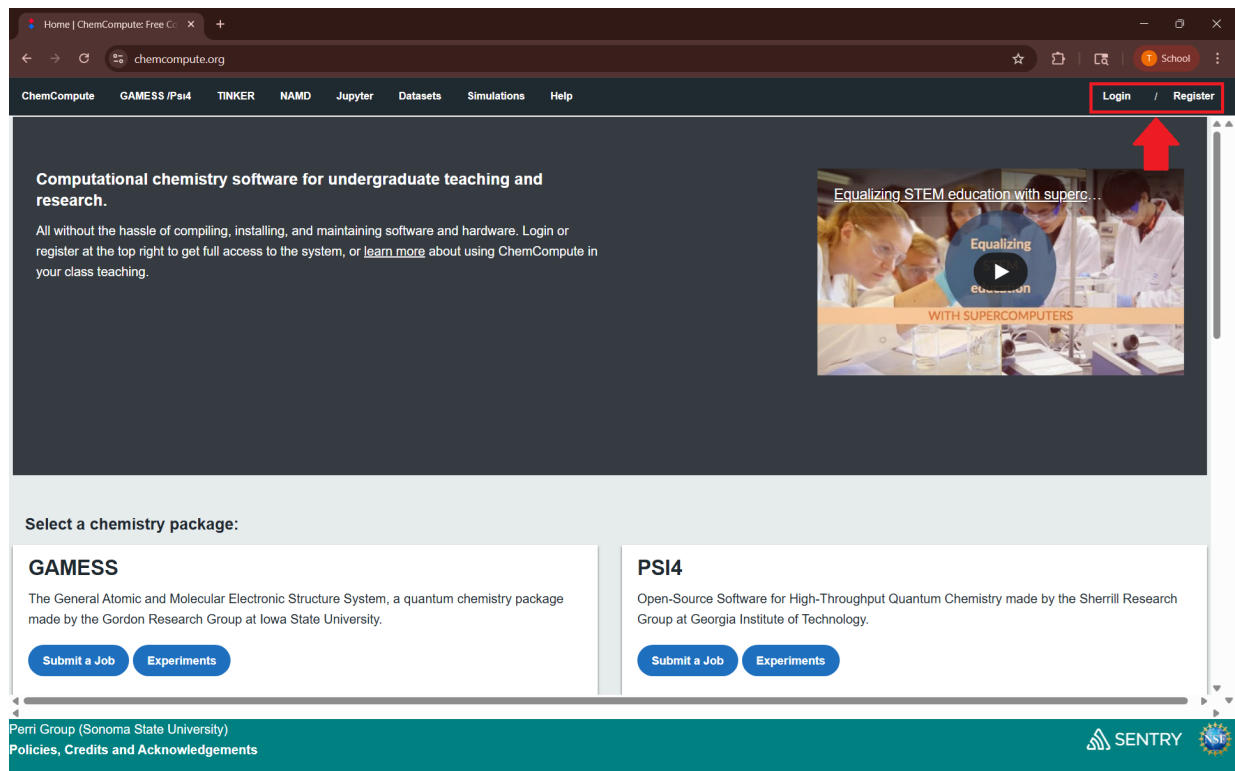
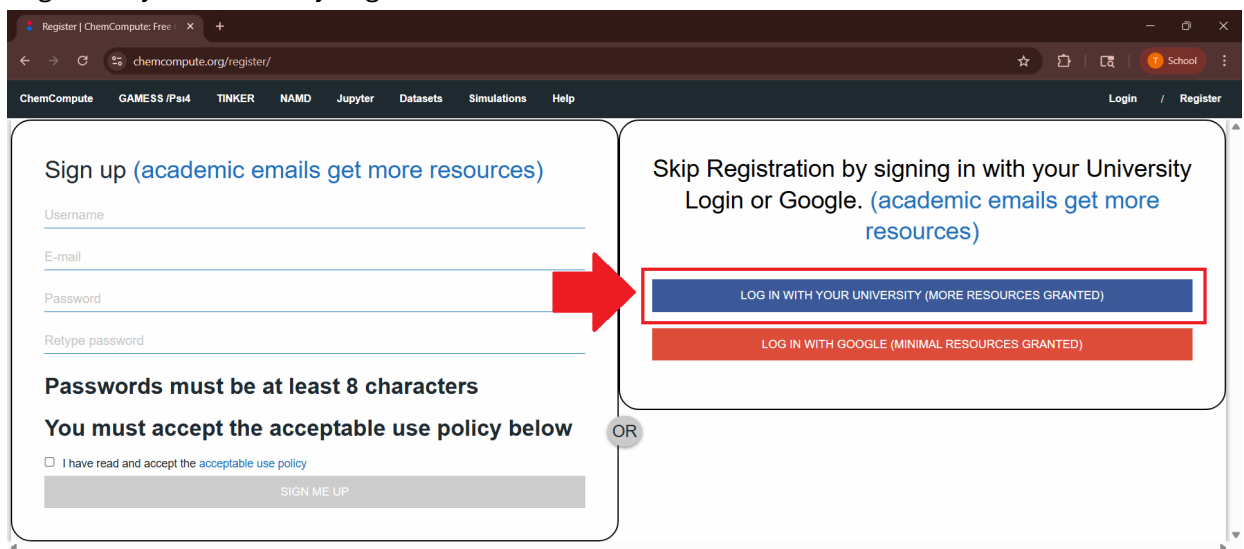


## Document 1: Getting Started

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 University from the dropdown menu.

Welcome To The CILogon Open

cilogon.org/authorize?response\_type=code&scope=openid+email+profile+org.cilogon.userinfo&client\_id=myproxy%3Aoa4mp%2C2012%3A%2Fclient\_id%2F251c447c13457...

**CILogon**

[Consent to Attribute Release](#)

chemcompute requests access to the following information. If you do not approve this request, do not proceed.

- Your CILogon user identifier
- Your name
- Your email address
- Your username and affiliation from your identity provider

**Select an Identity Provider**

Sonoma State University

☐ Remember this selection

Log On

By selecting "Log On", you agree to the [privacy policy](#).

For questions about this site, please see the FAQs or send email to [help@cilogon.org](mailto:help@cilogon.org).  
Know your responsibilities for using the CILogon Service.  
See acknowledgements of support for this site.

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

Home | ChemCompute: Free C...

chemcompute.org

ChemCompute GAMESS/PSI4 TINKER NAMD **Jupyter** Datasets Simulations Help

Tanner's Dashboard

**Computational chemistry software for undergraduate teaching and research.**

All without the hassle of compiling, installing, and maintaining software and hardware. Login or register at the top right to get full access to the system, or [learn more](#) about using ChemCompute in your class teaching.

Equalizing STEM education with supercomputers

WITH SUPERCOMPUTERS

**Select a chemistry package:**

**GAMESS**

The General Atomic and Molecular Electronic Structure System, a quantum chemistry package made by the Gordon Research Group at Iowa State University.

Submit a Job Experiments

**PSI4**

Open-Source Software for High-Throughput Quantum Chemistry made by the Sherrill Research Group at Georgia Institute of Technology.

Submit a Job Experiments

Perri Group (Sonoma State University)  
Policies, Credits and Acknowledgements

SENTRY NSF

6. Select “clone a repo from github”.

Jupyterhub / Jupyter Notebooks

Jupyterhub is a server for Jupyter Notebooks, which let users run python scripts through a web terminal.

### How does Psi4 / JUPYTERHUB work?

- 1 From the top menu select **Jupyter -- Use Jupyter Notebook**
- 2 **Clone a repo from github**
- 3 To generate a link for your students to automatically pull a repo from github use [This nbgitpuller link generator](#)

### Resource Limits / Quotas

- Each user is limited to 4 cores CPU and 6 GB RAM usage
- GPU nodes share a 40 GB A100 GPU between 1-5 users
- Users have a 12.5 GB disk quota in their ~ directory
- Users have a 5 GB disk quota in their ~/work directory. If you can't start a Jupyter Notebook it may be due to disk quota. Email me for an increase: [perrim@sonoma.edu](mailto:perrim@sonoma.edu)
- Only ~/work is preserved between sessions. ~ is ephemeral and will be reset when you stop / start your container

### Installed Packages Include:

- Python, R, and Julia
- Psi4
- PySCF and GPU4PySCF
- OpenMM and MDAnalysis

### JUPYTERHUB Experiments (20)

- Physical Chemistry
- General Chemistry
- General Instructions
- Analytical Chemistry
- Mathematics
- Electricity and Magnetism
- Machine Learning

Perri Group (Sonoma State University)  
Policies, Credits and Acknowledgements

SENTRY

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

Launch a Jupyter Notebook from: x +

chemcompute.org/jupyterhub/git

ChemCompute GAMESS /Psi4 TINKER NAMD Jupyter Datasets Simulations Help Hide Instructions Tanner'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 **Jupyter Notebook (default)** **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)”, then press start.

Launch a Jupyter Notebook from: JupyterHub

chemcompute.org/jupyterhub\_internal/hub/spawn

jupyterhub Home Token 3e9201cccd9c4678b37b57e44a7b0c86 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

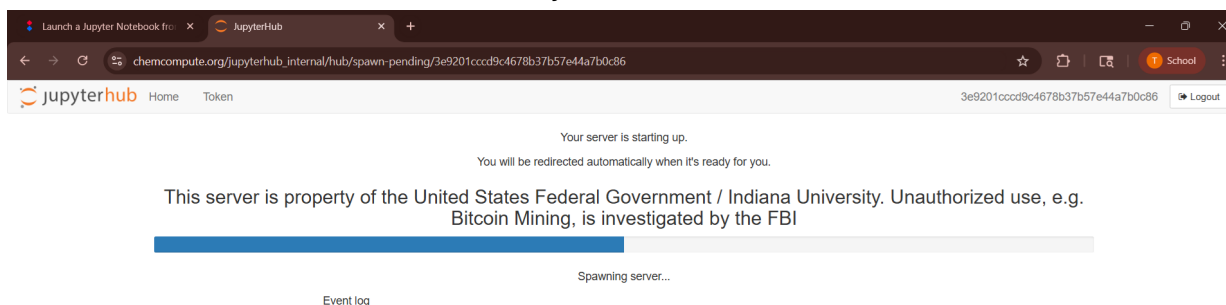
Select between Images

1.13 (Feb 25) -- Install pdb2pqr, meeko, prolif, pdbfixer, adme-py, smilite, Update pandas=2.2.3, openmm=8.2.0

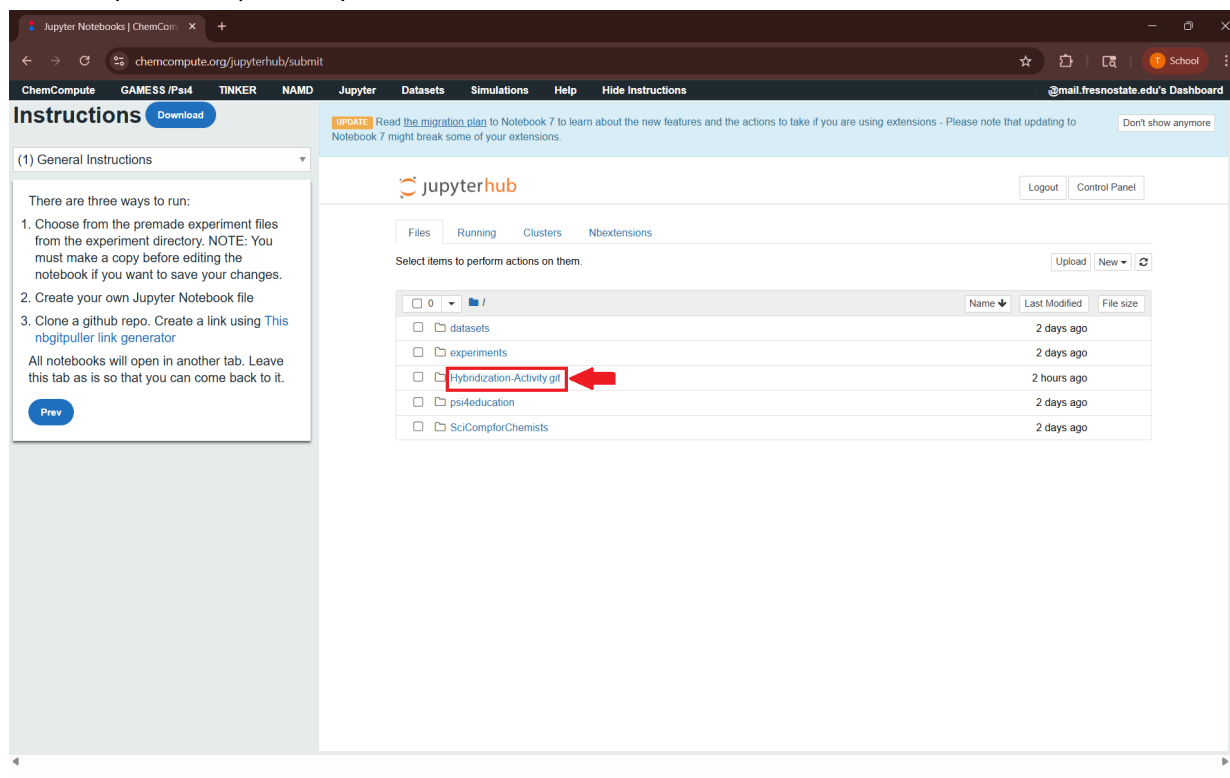
Julia 1.5.3, Python 3.11.9, R 4.3.3

Start

9. You will be redirected to a new tab. This may take a minute or two to load.



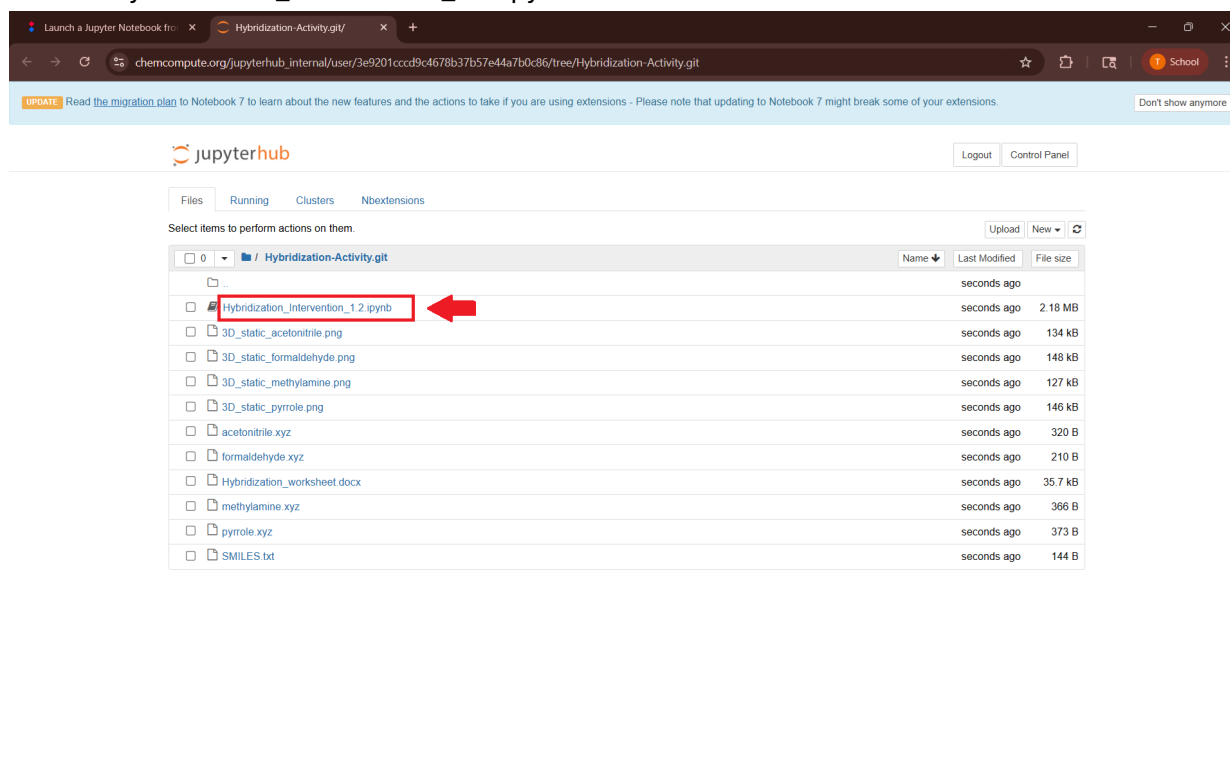
10. Once loading is complete, press Hybridization-Activity.git. If this folder does not show up, click on the tap from step 7 and repeat steps 7 – 9.



The screenshot shows the Jupyter Notebook interface. On the left, there is a sidebar with 'Instructions' and a 'Download' button. The main area displays the file explorer. The 'Hybridization-Activity.git' folder is highlighted with a red box, and a red arrow points to it. The file explorer shows a list of files and folders:

Name	Last Modified	File size
datasets	2 days ago	
experiments	2 days ago	
Hybridization-Activity.git	2 hours ago	
psi4education	2 days ago	
SciCompforChemists	2 days ago	

11. Select “Hybridization\_Intervention\_1.2.ipynb”. You will be redirected to one more tab.



The screenshot shows the Jupyter Notebook interface. The file explorer displays a list of files and folders within the 'Hybridization-Activity.git' directory. The 'Hybridization\_Intervention\_1.2.ipynb' file is highlighted with a red box, and a red arrow points to it. The file explorer shows a list of files and folders:

Name	Last Modified	File size
Hybridization_Intervention_1.2.ipynb	seconds ago	2.18 MB
3D_static_acetonitrile.png	seconds ago	134 kB
3D_static_formaldehyde.png	seconds ago	148 kB
3D_static_methylamine.png	seconds ago	127 kB
3D_static_pyrrole.png	seconds ago	146 kB
acetonitrile.xyz	seconds ago	320 B
formaldehyde.xyz	seconds ago	210 B
Hybridization_worksheet.docx	seconds ago	35.7 kB
methylamine.xyz	seconds ago	366 B
pyrrole.xyz	seconds ago	373 B
SMILES.txt	seconds ago	144 B

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

Launch a Jupyter Notebook from: x Hybridization-Activity.git/ x Hybridization\_Intervention\_1.2 x +

chemcompute.org/jupyterhub\_internal/user/3e9201cccd9c4678b37b57e44a7b0c86/notebooks/Hybridization-Activity.git/Hybridization\_Intervention\_1.2.ipynb

UPDATE Read the [migration plan](#) to Notebook 7 to learn about the new features and the actions to take if you are using extensions - Please note that updating to Notebook 7 might break some of your extensions. Don't show anymore

jupyterhub Hybridization\_Intervention\_1.2 (autosaved) Logout Control Panel

File Edit View Insert Cell Kernel Widgets Help Not Trusted Python 3 (ipykernel) Memory: 322.9 MB / 6 GB

### 3. Jupyter Notebooks and Color Scheme Explained

Jupyter notebook is a free open-source software that allows users to share computational documents, which is what this document is. We will be using the computational method of modeling, which is the act of creating a visual representation of a complex system, to support our understanding of said system. The system in question today is hybridization.

As you can see, sections are color-coded. Information that is meant to be read will be in this grey color.

Sections that will require you to type a response will be in this green color.

Sections that will require you to answer on the worksheet will be in this yellow color

And sections that will require you to code or execute a cell will be in this blue color.

You may have noticed you can click on the cells and see some texts with code, but cannot change anything. This is a useful feature to have for general applications of Jupyter notebook, but not as useful for our purposes. When you click on cells that can't be changed, just execute the cell (press the shift and enter key simultaneously) and move on the next cell.

