

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).

A screenshot of a web browser displaying the ChemCompute homepage at chemcompute.org/. The page features a dark header with navigation links for ChemCompute, GAMESS /Psi4, TINKER, NAMD, Jupyter, Datasets, Simulations, and Help. On the right side of the header, there is a "Login / Register" button, which is highlighted with a red arrow. Below the header, there is a banner with the text "Computational chemistry software for undergraduate teaching and research." and a subtext about equalizing STEM education with supercomputers. A video thumbnail is also visible. The main content area is titled "Select a chemistry package:" and lists two options: "GAMESS" and "PSI4", each with a "Submit a Job" and "Experiments" button. At the bottom of the page, there is a footer with links for "Perri Group (Sonoma State University)", "Policies, Credits and Acknowledgements", and logos for SENTRY and NSF.

3. Login with your University Login.

A screenshot of a web browser displaying the ChemCompute registration page at chemcompute.org/register/. The page has a similar header and navigation menu as the homepage. The main content is divided into two sections. The left section, labeled "Sign up (academic emails get more resources)", contains fields for "Username", "E-mail", "Password", and "Retype password". Below these fields, there is a note: "Passwords must be at least 8 characters" and "You must accept the acceptable use policy below". A checkbox for accepting the policy is present, followed by a "SIGN ME UP" button. A large red arrow points from this section to the right section. The right section, labeled "Skip Registration by signing in with your University Login or Google. (academic emails get more resources)", contains two buttons: "LOG IN WITH YOUR UNIVERSITY (MORE RESOURCES GRANTED)" and "LOG IN WITH GOOGLE (MINIMAL RESOURCES GRANTED)". A circular "OR" button is located between the two sections.

4. Select your University from the dropdown menu.

The screenshot shows a web browser window for 'Welcome To The CILogon Open'. The title bar says 'Welcome To The CILogon Open' and the URL is 'cilogon.org/authorize?response_type=code&scope=openid+email+profile+org.cilogon.userInfo+client_id=myproxy%3Aoa4mp%2C2012%3A%2Fclient_id%2F251c47c13457...'. The main content is titled 'Consent to Attribute Release' with a sub-section 'Select an Identity Provider'. A red arrow points to a dropdown menu where 'Sonoma State University' is selected. Below the dropdown is a checkbox for 'Remember this selection' and a 'Log On' button. At the bottom, there's a note: 'By selecting "Log On", you agree to the [privacy policy](#)'.

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

The screenshot shows a web browser window for 'Home | ChemCompute: Free Cr...' with the URL 'chemcompute.org'. The top navigation bar includes 'ChemCompute', 'GAMESS /Psi4', 'TINKER', 'NAMD', 'Jupyter' (which is highlighted with a red box and has a red arrow pointing to it), 'Datasets', 'Simulations', and 'Help'. The main content area features a banner with the text 'Computational chemistry software for undergraduate teaching and research.' and '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.' To the right of the banner is a video thumbnail with the text 'Equalizing STEM education with super...' and 'WITH SUPERCOMPUTERS'. Below the banner, there are two sections: 'GAMeSS' and 'Psi4'. Both sections have a 'Submit a Job' and 'Experiments' button. The footer contains links to 'Peri Group (Sonoma State University)', 'Policies, Credits and Acknowledgements', and logos for 'SENTRY' and 'NSF'.

6. Select “clone a repo from github”.

Jupyterhub / Jupyter Notebooks

How does Psi4 / JUPYTERHUB work?

- 1 From the top menu select Jupyter -- Use Jupyter Notebook
- 2 **Clone a repo from github** [Red arrow]
- 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
- 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

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

SENTRY NSF

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

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: [Red arrow]

Optional: enter branch (if not master or main)

Optional: choose between Jupyter Notebook (default) [Red arrow]
Notebook (default) or Jupyter Lab

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.

The screenshot shows a web browser window titled "JupyterHub" with the URL "chemcompute.org/jupyterhub_internal/hub/spawn". The page is titled "Server Options". It contains several configuration options:

- A note about GPU vs CPU node performance.
- A dropdown for "Select an instance for your notebook" set to "CPU node (default)".
- A dropdown for "Select between Jupyter Notebook and Jupyter Lab" set to "Jupyter Notebook (default)".
- A section for "Select a language" with radio buttons for Python (selected), R, and Julia.
- A section for "Select how to provide the image":
 - A radio button for "Select a Premade Image (default)" (selected).
 - A radio button for "Use a custom repository. These must be preapproved".
- A "Select between Images" dropdown showing "1.13 (Feb 25) – Install pdb2pqr, meeko, prolif, pdbfixer, adme-py, smilite. Update pandas=2.2.3, openmm=8.2.0".
- A "Julia 1.5.3, Python 3.11.9, R 4.3.3" link.

A large red arrow points upwards from the bottom of the page towards the "Start" button, which is highlighted with a red border.

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

The screenshot shows a web browser window titled "JupyterHub" with the URL "chemcompute.org/jupyterhub_internal/hub/spawn-pending/3e9201cccd9c4678b37b57e44a7b0c86". The page displays the following text:

Your server is starting up.
You will be redirected automatically when it's ready for you.

This server is property of the United States Federal Government / Indiana University. Unauthorized use, e.g. Bitcoin Mining, is investigated by the FBI

A progress bar at the bottom is labeled "Spawning server...".

A small "Event log" link is visible below the progress bar.

A large red arrow points upwards from the bottom of the page towards the progress bar.

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

The screenshot shows a web-based Jupyter Notebook interface. On the left, there is a sidebar titled "Instructions" with a "Download" button. The main content area shows a file list for a repository named "Hybridization-Activity.git". The file list includes:

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

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

The screenshot shows a web-based Jupyter Notebook interface. The user has navigated into the "Hybridization-Activity.git" folder. The file list includes:

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_pyrrrole.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
pyrrrole.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.

The screenshot shows a Jupyter Notebook interface. At the top, there are three tabs: 'Launch a Jupyter Notebook from...', 'Hybridization-Activity.git/...', and 'Hybridization_Intervention_1.2'. The main window title is 'jupyterhub Hybridization_Intervention_1.2 (autosaved)'. The toolbar includes File, Edit, View, Insert, Cell, Kernel, Widgets, Help, and various execution and cell management icons. A status bar at the bottom right shows 'Not Trusted', 'Python 3 (ipykernel)', and 'Memory: 322.9 MB / 6 GB'. The main content area contains a section titled '3. Jupyter Notebooks and Color Scheme Explained'. Below this, several colored boxes explain the color coding: grey for text meant to be read, green for sections requiring a response, yellow for sections requiring an answer, blue for sections requiring code or execution, and purple for notes about interacting with cells.

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.

13. Copy the website at the top. This will be placed into your worksheet.

