

Document 1: Getting Started

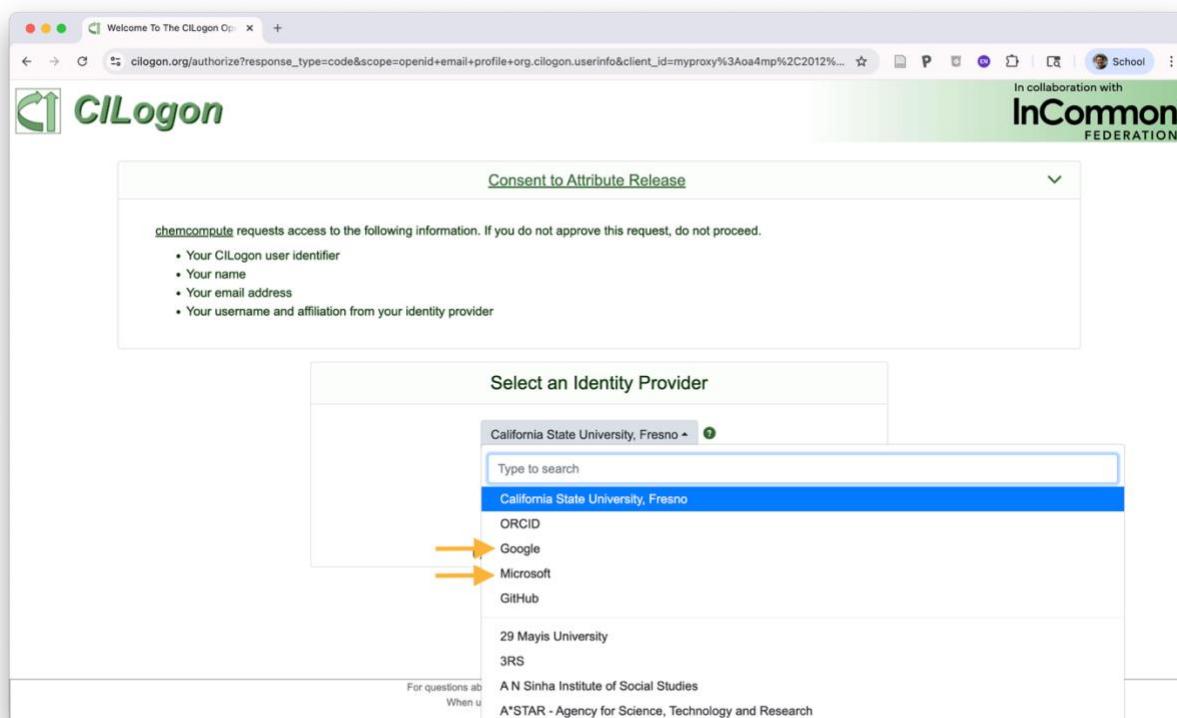
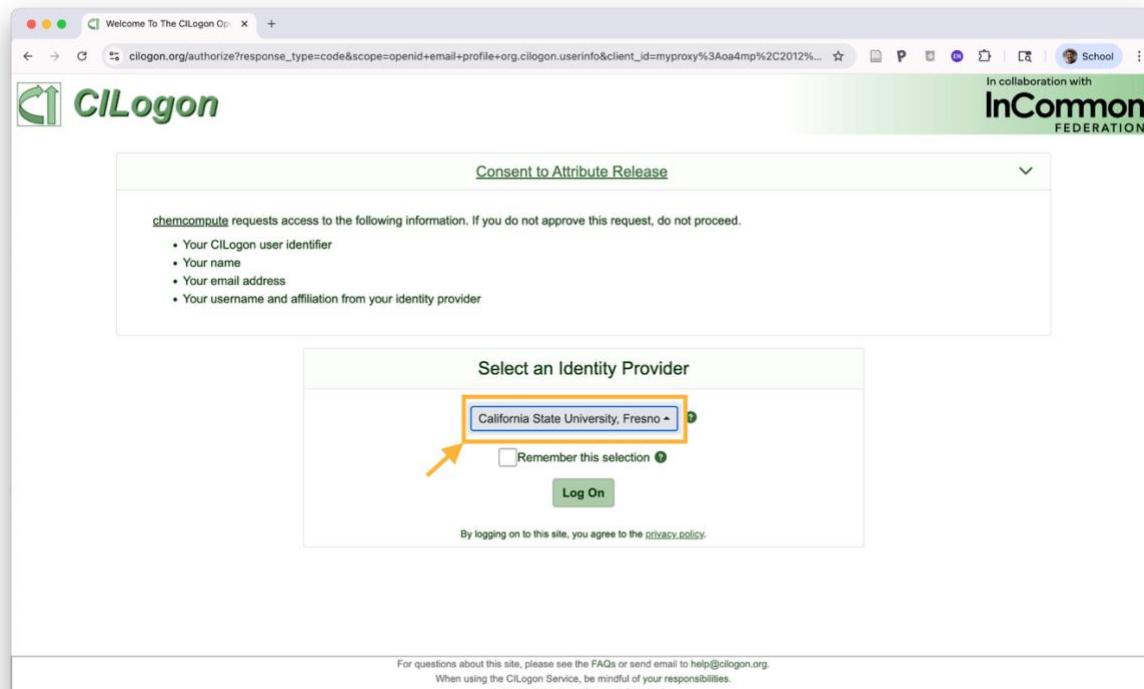
1. In your web browser, look up ChemCompute or enter this link into your address bar <https://chemcompute.org/>.
2. If you do not have an existing account with ChemCompute, you will need to register for one now (this is free).

The screenshot shows the ChemCompute homepage. At the top right, there are 'Login' and 'Register' buttons. A yellow arrow points to the 'Register' button. Below the header, there's a section titled 'Computational chemistry software for undergraduate teaching and research'. It lists four packages: GAMESS, Psi4, TINKER, and NAMD, each with a 'Submit a Job' button and an 'Experiments' button. At the bottom left, there's a footer with links to 'Perri Group (Sonoma State University)', 'Policies', 'Credits and Acknowledgements', and the URL 'https://chemcompute.org/register/'. On the right side, there are logos for 'SENTRY' and 'NSF'.

3. Login with your University Login.

The screenshot shows the 'Register' page of the ChemCompute website. It has two main sections. The left section is for 'Sign up', asking for a 'Username' and 'E-mail', and providing fields for 'Password' and 'Retype Password'. It also includes a note about passwords being at least 8 characters and accepting the 'acceptable use policy'. The right section is for 'Skip Registration by signing in with your University Login', featuring a 'LOG IN WITH YOUR UNIVERSITY (MORE RESOURCES GRANTED)' button. A yellow arrow points to this button. Below it, there's a note for users whose university uses Google or Microsoft for email. At the bottom, there's a 'SIGN ME UP' button and a checkbox for accepting the 'acceptable use policy'. The URL 'https://chemcompute.org/register/' is visible at the bottom left.

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”.



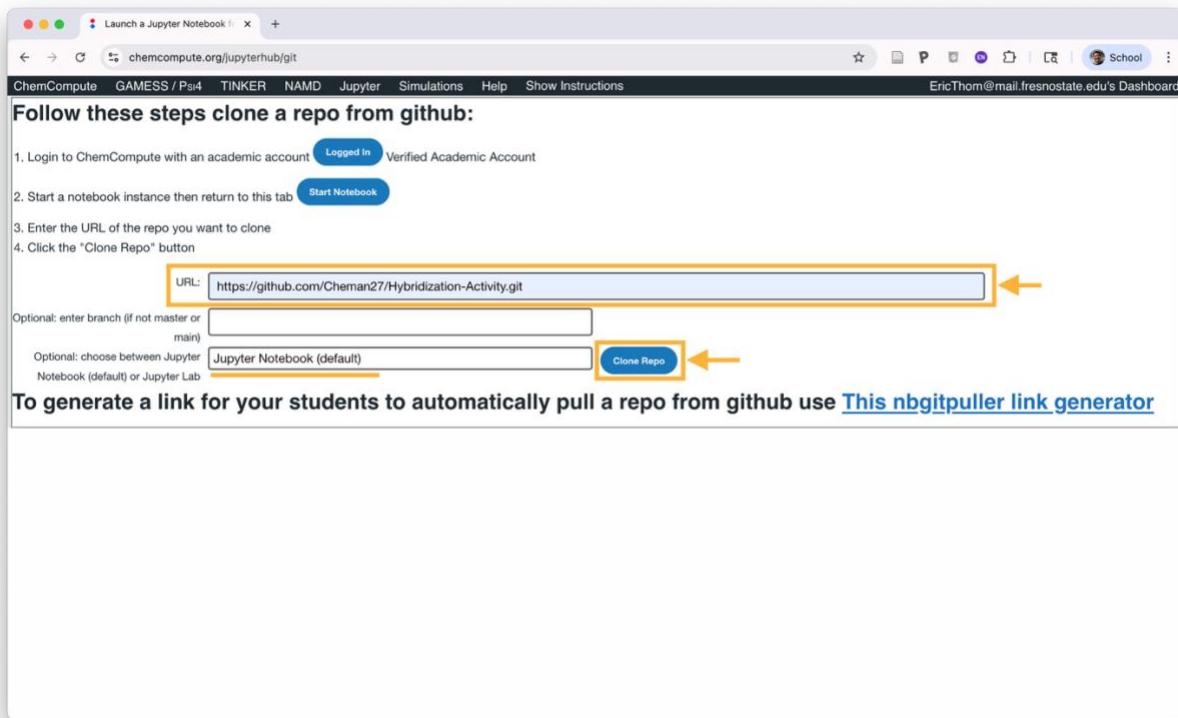
5. Select Jupyter (Dropdown menu when hovering is not relevant).

The screenshot shows the ChemCompute homepage. At the top, there is a navigation bar with links for ChemCompute, GAMESS / Psi4, TINKER, NAMD, Jupyter (which is highlighted with a yellow box and has an orange arrow pointing to it), Simulations, and Help. To the right of the navigation bar is a "Eric's Dashboard" link. Below the navigation bar, the page title is "Computational chemistry software for undergraduate teaching and research". A sub-header says "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." There are four main sections: GAMESS, PSI4, TINKER, and NAMD. Each section has a brief description, two blue buttons ("Submit a Job" and "Experiments"), and a "Perri Group (Sonoma State University)" link at the bottom.

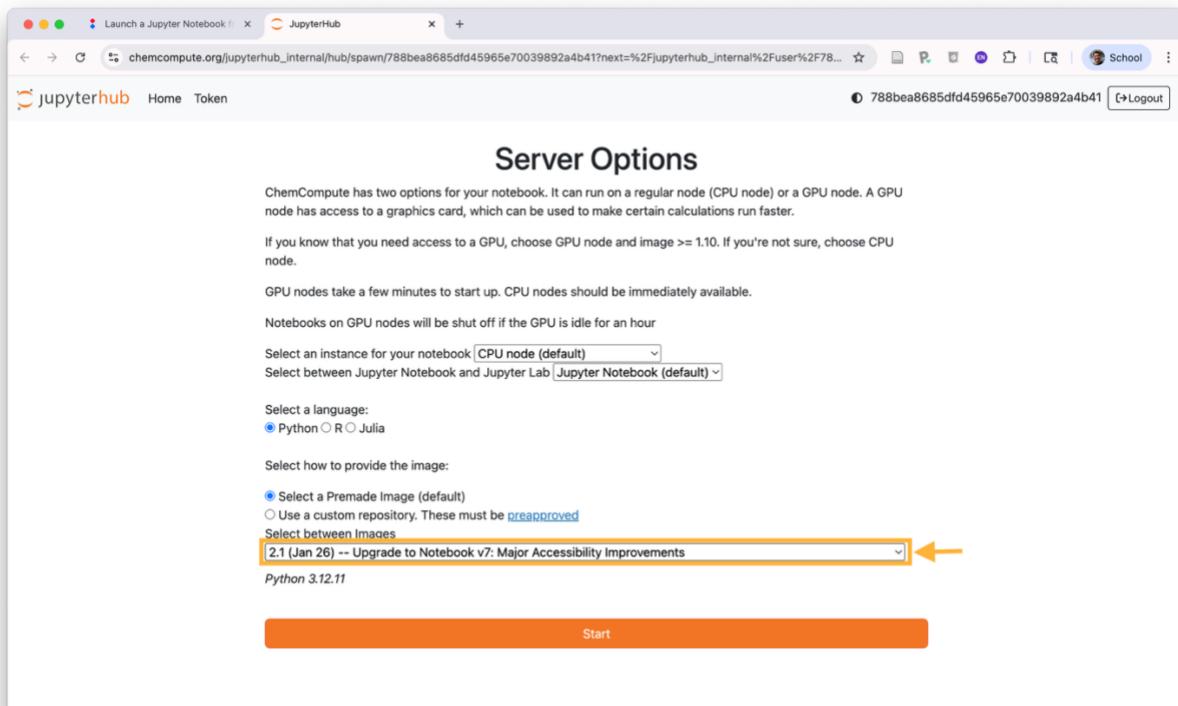
6. Select “clone a repo from github”.

The screenshot shows the Jupyterhub page. The top navigation bar includes links for ChemCompute, GAMESS / Psi4, TINKER, NAMD, Jupyter (highlighted with a yellow box and an orange arrow pointing to it), Simulations, and Help. The user is EricThom@mail.fresnostate.edu's Dashboard. The main content area is titled "Jupyterhub / Jupyter Notebooks" and contains the following sections: "How does Psi4 / JUPYTERHUB work?", "Resource Limits / Quotas", "Installed Packages Include:", and "JUPYTERHUB Experiments (20)". The "How does Psi4 / JUPYTERHUB work?" section lists three steps: 1. From the top menu select [Jupyter -- Use Jupyter Notebook](#), 2. **Clone a repo from github** (highlighted with a yellow box and an orange arrow pointing to it), and 3. To generate a link for your students to automatically pull a repo from github use [This nbgritpuller link generator](#) (opens in a new tab). The "Resource Limits / Quotas" section lists several bullet points about usage limits. The "Installed Packages Include:" section lists Python, R, and Julia. The "JUPYTERHUB Experiments (20)" section shows a list of categories with "+" icons to expand them: Physical Chemistry, General Chemistry, General Instructions, Analytical Chemistry, Mathematics, Electricity and Magnetism, and Machine Learning. The footer includes the "Perri Group (Sonoma State University)" link, "Policies, Credits and Acknowledgements", and SENTRY and NIST logos.

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



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.



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

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 [preapproved](#)

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 (selected)

1.15 (Oct 25) -- Added jupyter_mystr

1.14 (Apr 25) -- Added sweetviz, pandastools.

1.13 (Feb 25) -- Install pdb2pqr, meeko, prolf, pdbfixer, adme-py, smilite. 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.

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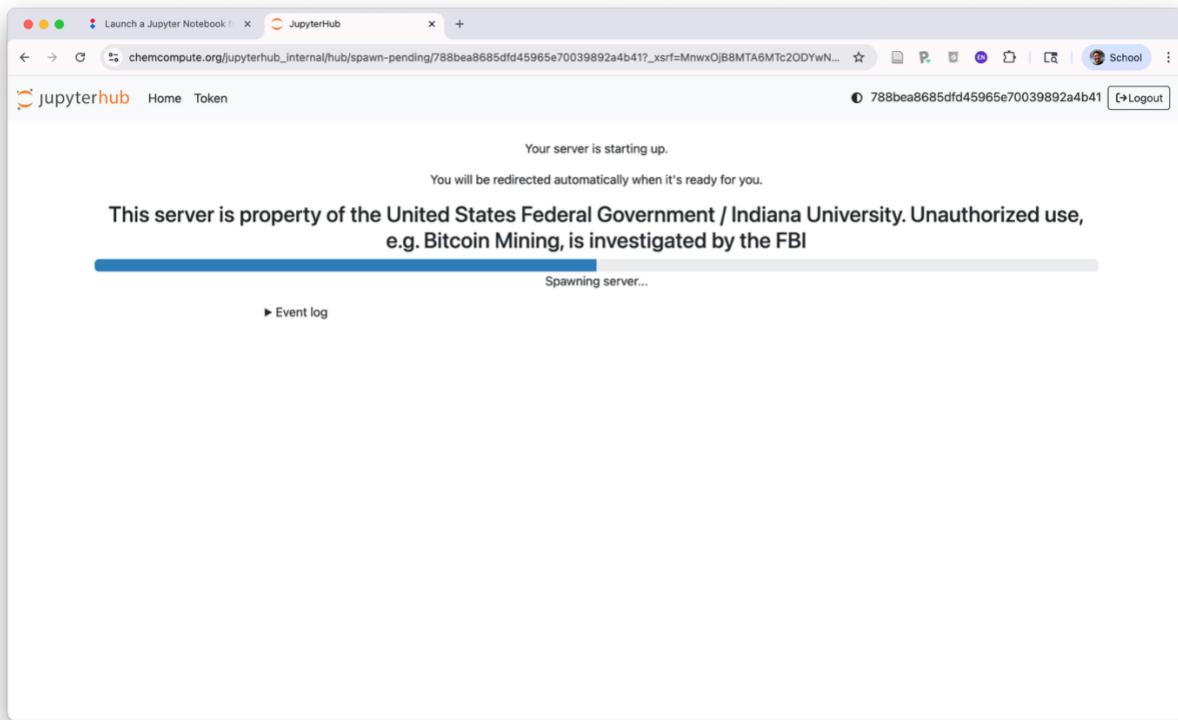
Select between Images

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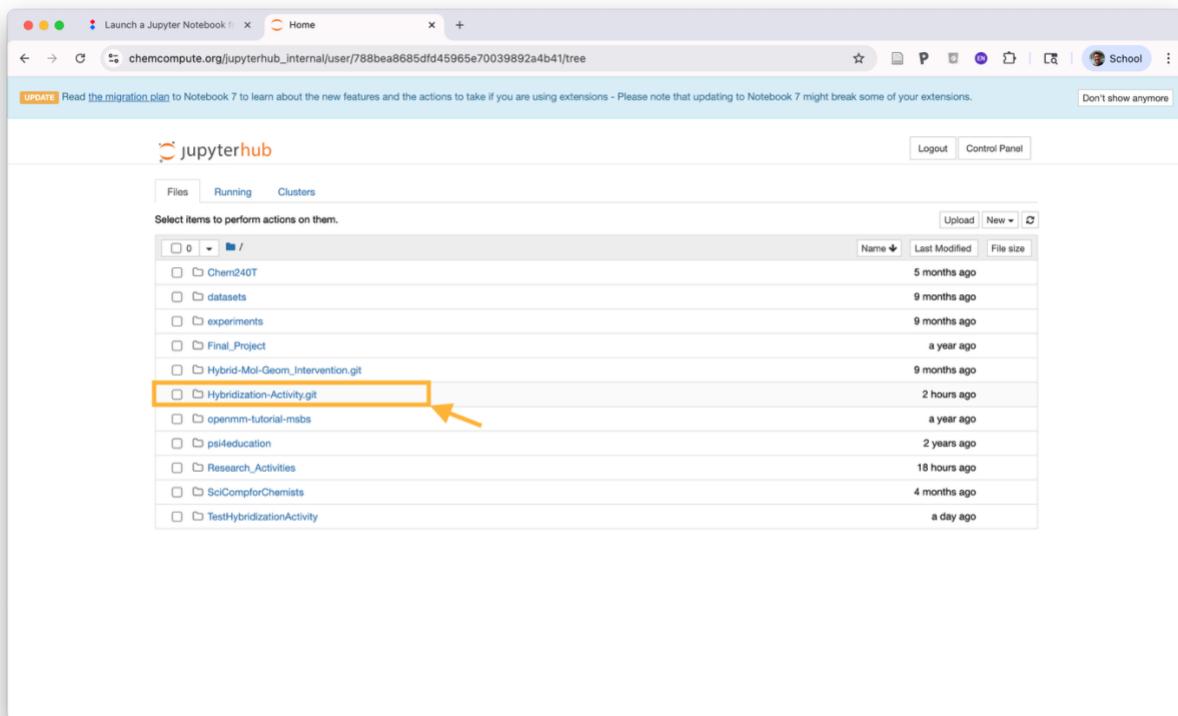
Python 3.12.11

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.

The screenshot shows a web browser window with the URL chemcompute.org/jupyterhub/internal/user/788bea8685dfd45965e70039892a4b41/tree/Hybridization-Activity.git. The page title is "jupyterhub". The main content is a file list under the path "/Hybridization-Activity.git". The file "Hybridization_Intervention_1.2.ipynb" is highlighted with a yellow box and an orange arrow pointing to it. The file list includes various files and folders such as "3D_static_acetonitrile.png", "3D_static_allene.png", "3D_static_allene_20251205234617.png", etc.

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

The screenshot shows a Jupyter Notebook interface with the title "Hybridization_Intervention_1.2 Last Checkpoint: 18 hours ago (unsaved changes)". The notebook content starts with a section titled "3. Jupyter Notebooks and Color Scheme Explained". The text explains that Jupyter notebook is a free open-source software that allows users to share computational documents, which is what this document is. It mentions 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. Below this, there is a note about sections being color-coded: "As you can see, sections are color-coded. Information that is meant to be read will be in this grey color." followed by "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 "And sections that will require you to code or execute a cell will be in this blue color.". At the bottom, there is a note about cells: "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."

