

Document 1: Getting Started

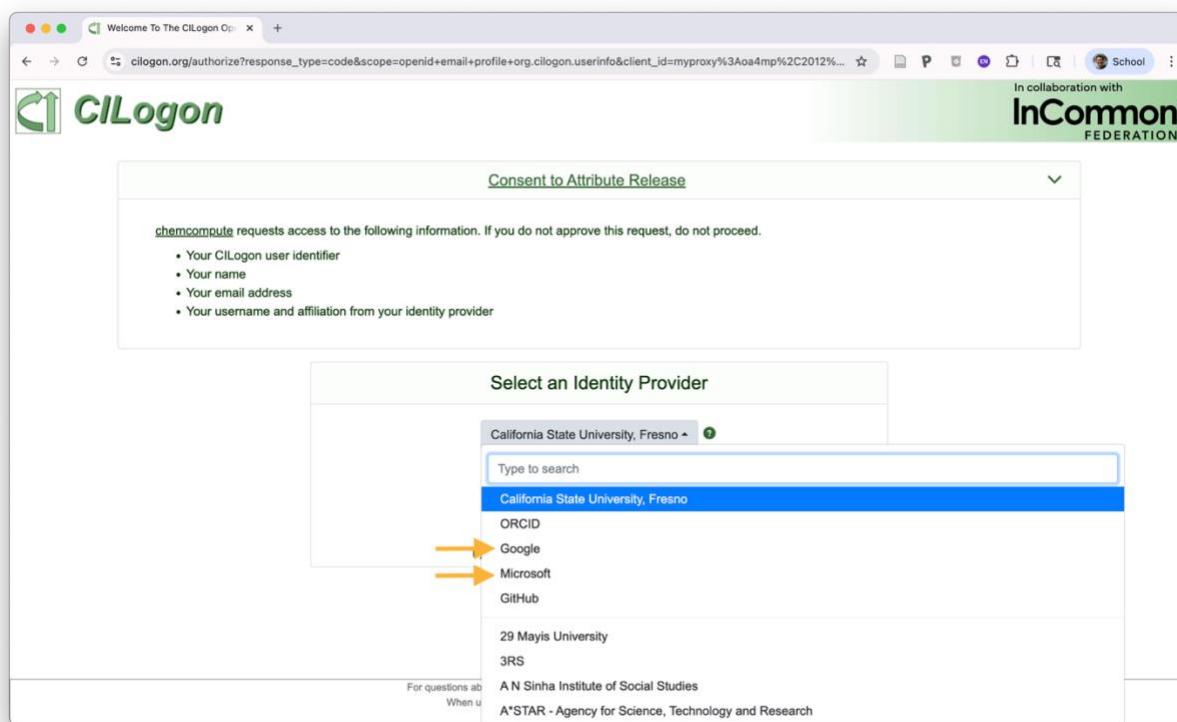
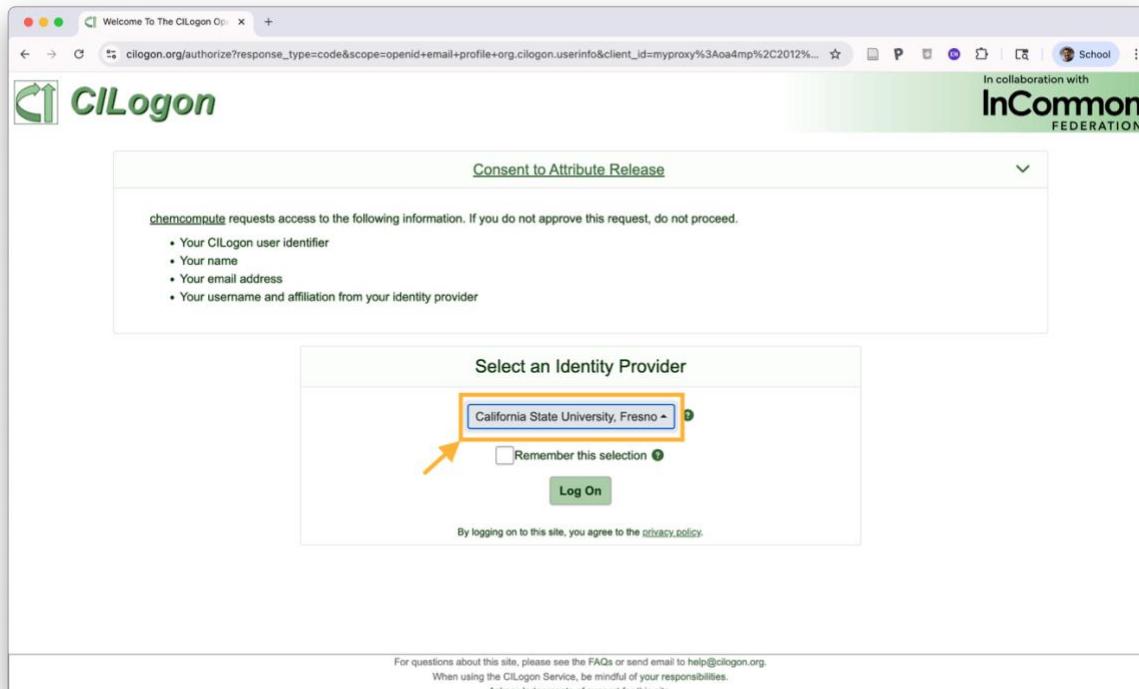
1. In your web browser, look up ChemCompute or enter this link into your address bar <https://chemcompute.org/>.
2. If you do not have an existing account with ChemCompute, you will need to register for one now (this is free).

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 chemistry packages: GAMESS, Psi4, TINKER, and NAMD. Each package has 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', which includes 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 website interface. 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, it says "Eric's Dashboard". Below the navigation bar, there is a section titled "Computational chemistry software for undergraduate teaching and research". This section contains four main categories: GAMESS, PSI4, TINKER, and NAMD. Each category has a brief description, a "Submit a Job" button, and an "Experiments" button. At the bottom of the page, there is a green footer bar with the text "Perri Group (Sonoma State University)", "Policies, Credits and Acknowledgements", and logos for SENTRY and NIST.

6. Select “clone a repo from github”.

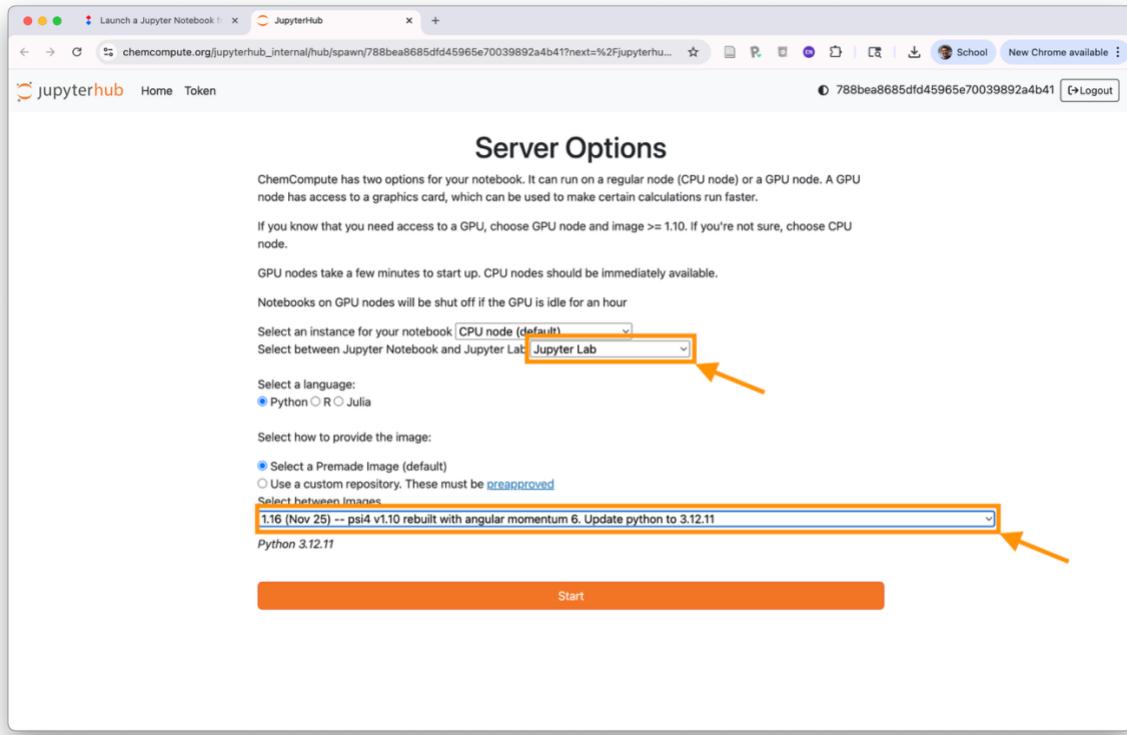
The screenshot shows the Jupyterhub / Jupyter Notebooks page. On the left side, there is a sidebar with the title "Jupyterhub / Jupyter Notebooks" and a description: "Jupyterhub is a server for Jupyter Notebooks, which let users run python scripts through a web terminal.". Below this, there is a section titled "How does Psi4 / JUPYTERHUB work?" with three numbered steps: 1. From the top menu select [Jupyter -- Use Jupyter Notebook](#), 2. [Clone a repo from github](#) (which is highlighted with a yellow box and has 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). There is also a section titled "Resource Limits / Quotas" with a bulleted list of usage details and contact information for perrim@sonoma.edu. On the right side, there is a section titled "JUPYTERHUB Experiments (20)" with a list of experiment categories: Physical Chemistry, General Chemistry, General Instructions, Analytical Chemistry, Mathematics, Electricity and Magnetism, and Machine Learning. At the bottom of the page, there is a green footer bar with the text "Perri Group (Sonoma State University)", "Policies, Credits and Acknowledgements", and logos for SENTRY and NIST.

7. Paste the URL <https://github.com/Cheman27/Hybridization-Activity.git> into the designated portion. Click on the menu option for “Optional: choose between Jupyter Notebook (default) or Jupyter Lab” and select “Jupyter Lab”, then select “Clone Repo” button.

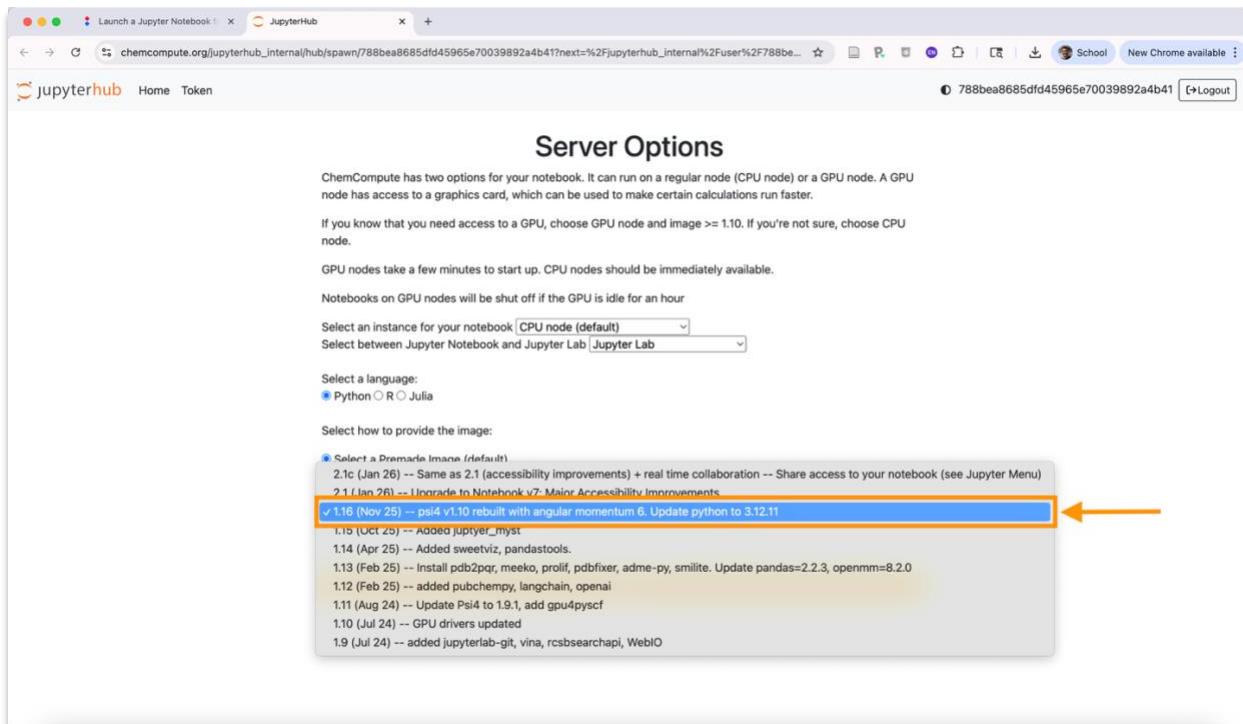
The screenshot shows a web browser window titled "Launch a Jupyter Notebook". The address bar contains "chemcompute.org/jupyterhub/git". The page header includes "ChemCompute", "GAMESS / Psi4", "TINKER", "NAMD", "Jupyter", "Simulations", "Help", "Show Instructions", and "EricThom@mail.fresnostate.edu's Dashboard". Below the header, a section titled "Follow these steps clone a repo from github:" lists four steps: 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, and 4. Click the "Clone Repo" button. Step 3 has a URL input field containing "https://github.com/Cheman27/Hybridization-Activity.git" highlighted with an orange box and an arrow pointing to it. Step 4 has a dropdown menu for "Optional: choose between Jupyter Notebook (default) or Jupyter Lab" with "Jupyter Lab" selected, also highlighted with an orange box and an arrow pointing to it. A blue "Clone Repo" button is visible at the bottom right of the dropdown menu. At the bottom of the page, a link "To generate a link for your students to automatically pull a repo from github use [This nbgitpuller link generator](#)" is displayed.

This screenshot is identical to the one above, showing the same interface and steps for cloning a GitHub repository. The URL "https://github.com/Cheman27/Hybridization-Activity.git" is entered in the URL field, and the "Jupyter Lab" option is selected in the dropdown menu. The "Clone Repo" button is highlighted with an orange box and an arrow pointing to it. The bottom link for generating a nbgitpuller link is also present.

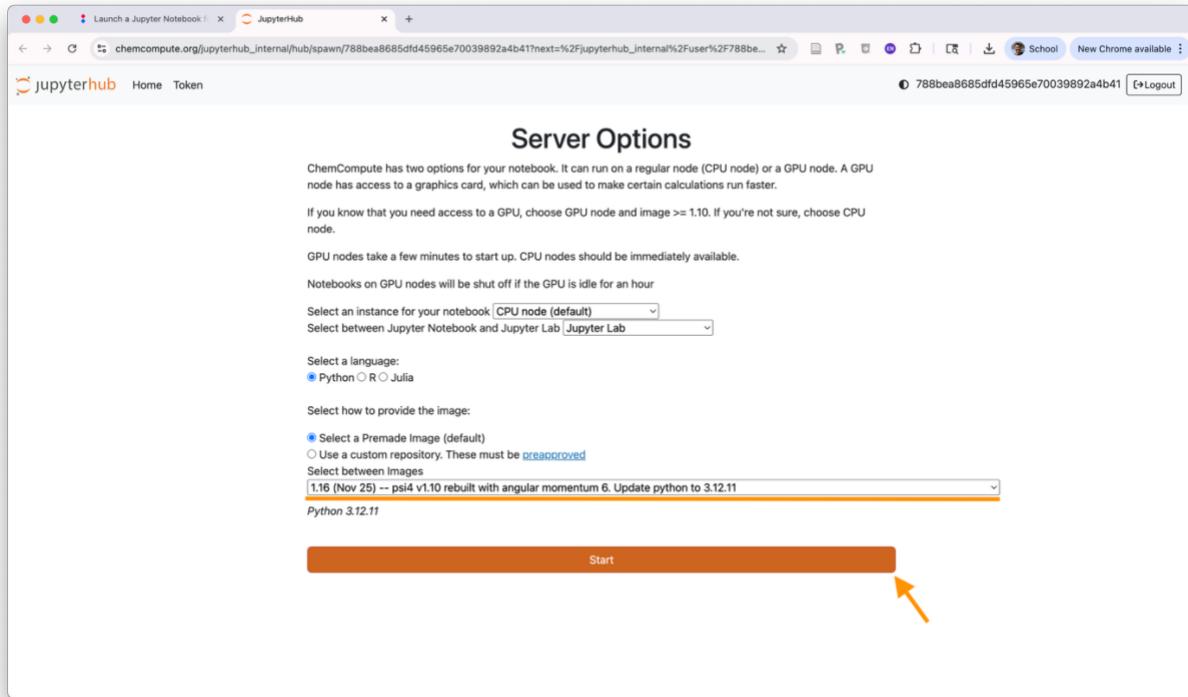
8. Once redirected, ensure “Select between Jupyter Notebook and Jupyter Lab” option is set to “Jupyter Lab”, and the “Select a language” option is set to “Python” and the “Select how to provide the image” option is set to “Select a Premade image (default)”, and lastly, you will need to change “Select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



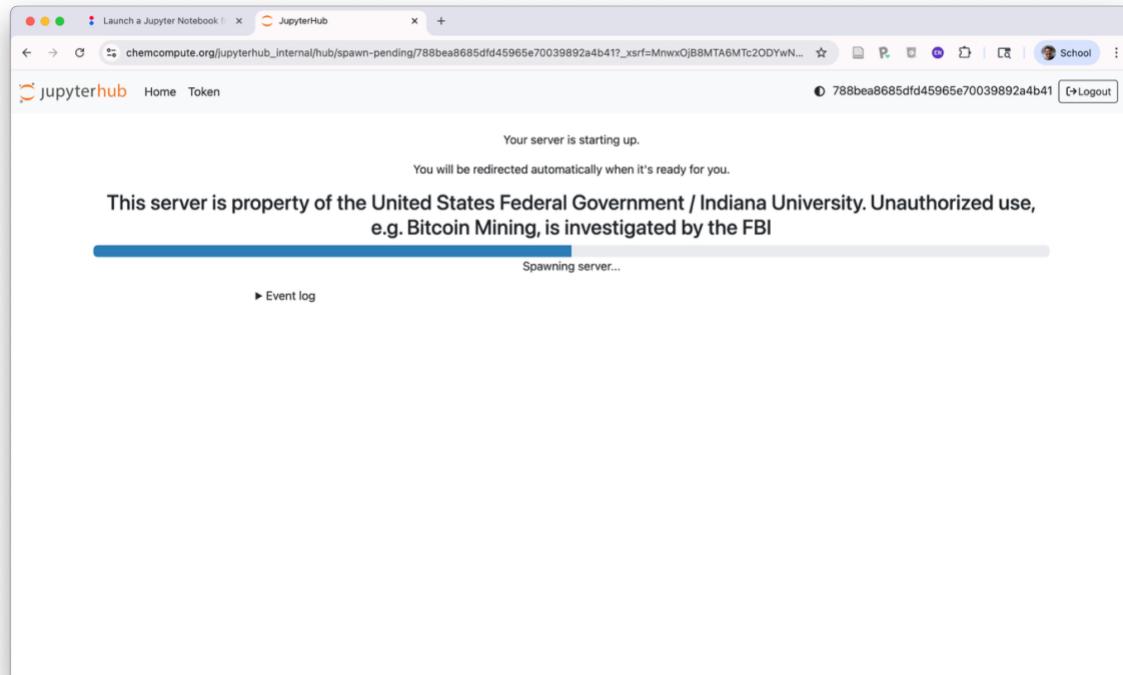
9. From the dropdown menu select “1.16 (Nov25) – psi4 v1.10rebuilt with angular momentum 6. Update python to 3.12.11”.



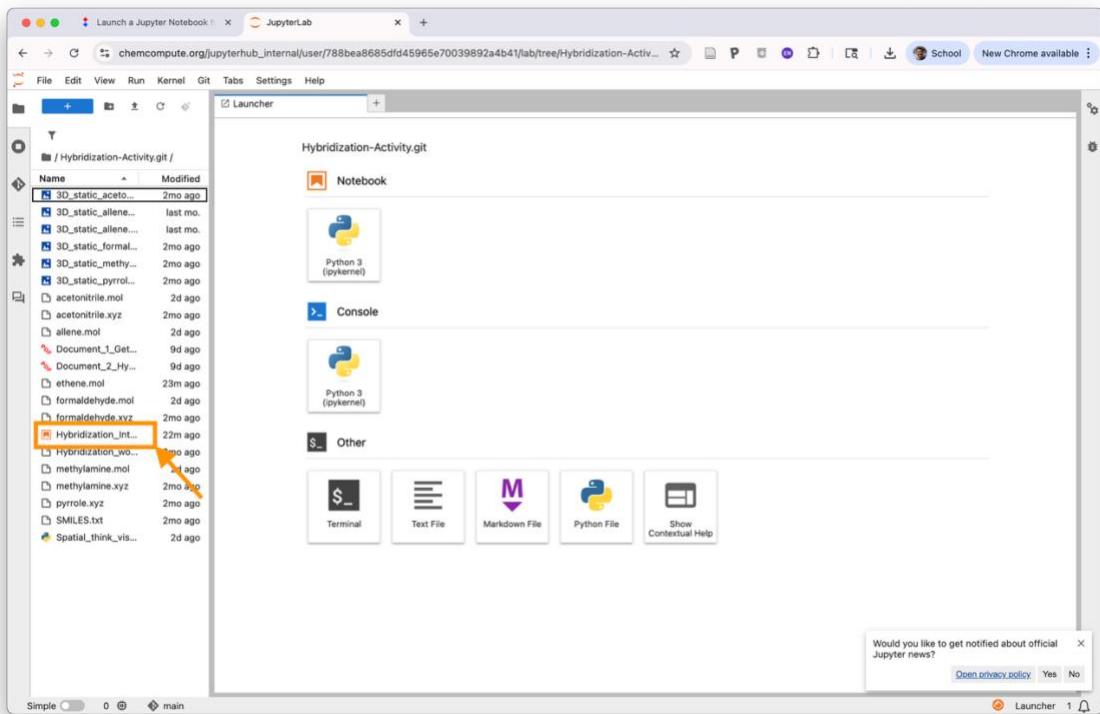
10. Now click Start.



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, click on Hybridization-Activity.git. Do not worry about clicking into any of the other files. It is only important that you interact with the Hybridization-Activity.git file.



13. The viewer window will open another tab. Now that you can access your jupyter notebook, **proceed to Document 2: Hybridization Worksheet**.

