Name: \_\_\_\_\_\_\_\_\_\_

Student ID#: \_\_\_\_\_\_\_\_\_\_

1. What to expect

Computational Chemistry is a discipline in the field of chemistry that investigates chemical phenomena (observable natural or human-made chemical events) with a computer. Computational Chemists use the computational power (ability to perform mathematical calculations) of a computer to investigate topics in chemistry, from molecular geometry to predicting spectra and many things in between. A unique ability the discipline of computational chemistry has is the ability to generate visual representations and models to aid in the understanding of chemical phenomena, which is what we will be using today to understand hybridization in the context of organic chemistry.

In this activity, you will be applying a computational method (modeling) to understand hybridization. You will not be tasked with learning how to code, but you will be tasked with knowing what to code and writing said code correctly (check the appendix, pages 5 and 6). The researchers have coded a set of functions for you to call.

Writing code requires typing with accuracy, so take your time when needed. Coding will require that you type every letter, symbol, and number exactly as the code was written. Throughout this worksheet, you will be introduced to coding terms, which are explained in the appendix section (Page 5).

1. What to do now

* Open your Jupyter notebook that was set up on your familiarization day. See the Getting Started worksheet for more information.
* Read through and follow the instructions outlined in the Jupyter notebook sequentially.

**5.1. Illustration Box 1**: To the best of your ability, draw a diagram of an s orbital, a p orbital, and a hybrid orbital. Once complete, or if you are struggling to recall this information, progress to the section in the activity titled “Short Coding Familiarity and Practice” in your Jupyter Notebook

**12. Illustration Box 2**: Please draw a diagram of Pyrrole. You need to include the hybridization state of nitrogen and specify which bonds are sigma 𝜎 and pi 𝜋. If lone pairs exist, you need to include those in your model.

Downloading and Submitting your Jupyter Notebook

**Appendix**

Terms and definitions

|  |  |
| --- | --- |
| **Terms / phrases (and variations)** | **Definition** |
| Computational method | The process of using tools from computer science to gain insights into a system of interest (like chemistry). |
| Function | reusable code that performs a specific task. |
| To call a function | This is the act of using a specific function (the part you will type). You will have to type the name of the function you want to use, followed by a set of parentheses. |
| Jupyter notebook | A free web service that allows users to write interactive code and share said code with others. |
| Cell | An interactive section in Jupyter notebook to write and execute code. |
| Execute | Activate blocks of code. In Jupyter notebook you must press the shift key and return key at the same time “shift+return” for mac users. For window users “shift+enter” |
| Bug | A flaw or error in code that results in unexpected results |
| Library | A collection of functions |
| Polarization | The separation of charge resulting in an uneven sharing of charge across the molecule |

|  |  |
| --- | --- |
| **Function** | **Action** |
| stv.example\_code\_s\_orbital() | Generates an s orbital on a carbon of ethane in a 3D-interactive representation |
| stv.example\_code\_p\_orbital() | Generates a p orbital on a carbon of ethane in a 3D-interactive representation |
| stv.view2D\_flat("methylamine") | Generates a flat 2D representation of methylamine |
| stv.view2D\_flat("formaldehyde") | Generates a flat 2D representation of formaldehyde |
| stv.view2D\_flat("acetonitrile") | Generates a flat 2D representation of acetonitrile |
| stv.view2D\_flat(“pyrrole”) | Generates a flat representation of pyrrole |
| stv.view2D\_depth\_methylamine() | Generates a 2D representation that implies depth of methylamine |
| stv.view2D\_depth\_formaldehyde() | Generates a 2D representation that implies depth of formaldehyde |
| stv.view2D\_depth\_acetonitrile() | Generates a 2D representation that implies depth of acetonitrile |
| stv.view2D\_depth\_pyrrole() | Generates a 2D representation that implies depth of pyrrole |
| stv.view3D\_static\_methylamine() | Generates a static 3D representation of methylamine |
| stv.view3D\_static\_formaldehyde() | Generates a static 3D representation of formaldehyde |
| stv.view3D\_static\_acetonitrile() | Generates a static 3D representation of acetonitrile |
| stv.view3D\_static\_pyrrole() | Generates a static 3D representation of pyrrole |
| stv.view3D\_int\_methylamine() | Generates an interactive 3D representation of methylamine |
| stv.view3D\_int\_formaldehyde() | Generates an interactive 3D representation of formaldehyde |
| stv.view3D\_int\_acetonitrile() | Generates an interactive 3D representation of acetonitrile |
| stv.view3D\_int\_pyrrole() | Generates an interactive 3D representation of pyrrole |

**Functions Table**