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

Student Id #: \_\_\_\_\_\_\_\_\_\_

Brief coding background information

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| **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 |

In this activity you will be applying computational methods to understand chemistry topics. 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. 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. You will also need to evaluate a few cells in order as they appear so you can call any of these functions later in the activity.

Illustration Box 1: Please draw a model of an s orbital, a p orbital, and a hybrid orbital

Illustration Box 2: Please draw a model 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.

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