**Amanda Dewyer**

**Basis Set Selector ReWoTe**

**EXABYTE.io Interview**

Overview:

The aim of this project is to develop a python package that allows for the automated selection of an appropriate basis set for quantum chemical calculations based on a user defined molecule.

Requirements

1. Automatically identify a basis set for a user defined chemical system within a given tolerance level.
2. Utilize previously published or high level (couple cluster) energies as reference data.
3. Have the ability to calculate a structure's energy using various basis sets and converge on a reference point energy.
4. It should be clear that the ability to expand this to other properties is straightforward and easy to implement in a future version of this code.

Expectations

1. Modular and object oriented programming using python.
2. Identify a basis set correctly for molecules ranging in size from 2-20 atoms.
3. Basis set demonstration should cover at least 5 unique structures with varying size.
4. The code will work for a variety of tolerance levels and return the most cost effective basis set. (i.e. larger tolerance range returns lower accuracy, more cost efficient, basis set.)

Timeline

* The project should take approximately 5 days to code.
* Demonstration of the code will be given on September 16th 2020.

User Story

The user should be able to pass the code the following parameters and in return be given a basis set that satisfies the criteria.

1. Molecular structure including charge and multiplicity
2. Reference energy (property value)
3. Level of theory (HF, DFT functional, etc.) for use in calculating properties with various basis sets.
4. Tolerance threshold for basis set selection

Notes

* If time permits I would like to demonstrate/implement a simple heuristics based basis set selector as well. It would work for small main group element molecules as a demonstration of the idea.
* The code will be written to work with NWChem.