

Step1: Load plotting-k-means.py into your IDE.

Step2: Feel free to edit Line8 (numcluster variable) to values between 3 to 6 before running the python script.

Step3: Running the python script will generate two 3D figures. The first plot is a scatter of all the atoms colored based on the clustering algorithm, plus an overlay of the centroids of each of the 'numclusters' clusters. The second plot a scatter of ONLY the centroids of the cluster.

## Example Figures

K-Means for numclusters=4

