# Assignment 2

- **All questions are of equal value.**
- **Important:** This assignment should be returned using GitHub. If you don't have an account, create a GitHub account, and in GitHub create a directory called Chem9664B. Make that directory private and share it with me. My username at GitHub is mejk (you need that for sharing). This assignment also assumes that you have now access to the command line terminal (Linux, WSL in Windows or Mac terminal), and have python and Jupyter Lab installed. Installation help is in the online course notes.
- **All of the tasks below should be in one single Jupyter notebook (ipynb file).**

Due: Friday Feb 10, 2023 at midnight.

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1. Write a small python program (in the Jupyter Lab environment) that reads attempts to insert particles of diameter 1 Å randomly in a 2-d simulation box (closed boundaries) of size 11 x 11 Å. Use uniformly generated random numbers.
a) What is the maximum density you can reach? Give the results using number density.
b) Plot also time it takes to generate a configuration as a function of number density. Important: you need to average over at least 10 attempts and plot error bars and report how the error bars were generated.

2. Use the parameters from above and write a code to generate an initial configuration based on a triangular (hexagonal) 2-d lattice.

3. In the lectures, a pseudo-code was given that shows how to count for interactions that have a cutoff than L/2 (assume that the system is a square). Assume that the strength of particle-particle interaction is independent of the distance and has a value of unity if within the cutoff and zero otherwise. Compute the total energy of the system in problem 2.