COS 701 Project 2

1. Write a computer program to calculate the potential energy and forces by using Keating potential (Phys. Rev. **145**, 637, 1966) on a silicon system, where N atoms are randomly distributed in a box of length L and each atom is four-fold coordinated. Assume that the mass density of the system is 2.30 gram/cm^3. Choose N = 1000 and fix L so that the experimental density given here is realized.

2. Minimize the potential energy of the system using Monte Carlo or any other optimization programs. You may use standard package programs from Matlab/Python or from equivalent software packages.

3. Plot the energy as a function of MC steps or iterations (for Newton methods, etc.)

4. Compare the forces obtained from the analytical expression of the Keating potential with those from numerical energy calculations.

5. Calculate the pair-correlation function, bond-angle distribution, and the coordination-number distribution to characterize the structures that you generate.