

## COS 701 Project 1

1. Write a computer program to calculate the potential energy and forces by using Stillinger-Weber (SW) potential (see class note and Phys. Rev. B **31**, 5262, 1985) on a silicon system, where  $N$  atoms are randomly distributed in a box of length  $L$ . Assume that the mass density of the system is  $2.30 \text{ gram/cm}^3$ . 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 SW 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.