Example Quiz #1
EE 539 Nanotechnology Modeling

1. Describe how you might estimate using MD the solubility as a function of temperature of a solute A in a matrix B at atmospheric pressure in the presence of competing A-rich phase AB. Your answer should specify initial conditions, boundary conditions, the ensemble used and how the desired quantities could be extracted from the results of MD runs. What could you do to help convince someone that your answer was correct (given empirical potential)?

2. The figure at right is correlation function from an MD run for two systems.
   a. Identify crystalline and amorphous structures.
   b. Give possible parameters for Lennard Jones (6-12) potential consistent with this plot.
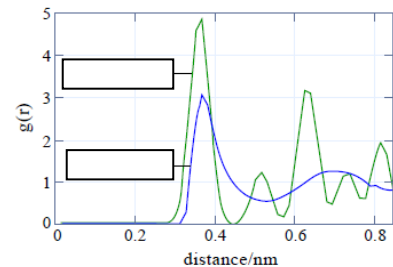
3. How would you use DFT calculations to calculate the ratio of solubility of substitutional Au in Si between temperatures of 700 and 1000°C [$C_{ss}(700°C)/C_{ss}(1000°C)$]? Assume the system of interest is Si wafer capped with thick fcc Au film. Specify the systems/conditions you would use, what you would extract from the calculations, and exactly how you would use those calculation results (give equation).