Name:_____

Quiz #2
EE 539C Nanotechnology Modeling
December 2, 2009

1. 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).

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2. You would like to use kinetic lattice Monte Carlo (KLMC) to calculate vacancy mediated interdiffusion (mixing of two alloy components) in AB fcc metal alloy as function of the composition. Assume you have available MD code with well-characterized empirical potential that can be used for calculating parameters and V concentration is very small.
    a. What calculations would you need to do to set up parameters for KLMC simulations of this system? Assume you have KLMC code which works on fcc lattice and that only 1NN interactions are significant.

    b. How would you initialize the system and what would you measure to quantify diffusivity as function of composition?

    c. How would normalize your results to be consistent with equilibrium vacancy concentration at temperature of interest?