EE539B
Nanotechnology Modeling
Fall 2015

Assignment #2
Due 10/29/15

Please prepare the assignment in the form of a technical report describing the calculations made (including any relevant equations), followed by the results. You should be able to make extensive use of the examples provided from the VASP Workshop as templates for your calculations. Post questions on GoPost when practical.

1. Use VASP to calculate the cohesive energy of greenhouse gas CO_2 relative to constituent atoms. Also extract from the calculation the equilibrium bond lengths and angles. Test for convergence in supercell size and energy cut-off using the LDA functional, then repeat calculation using GGA under the same conditions. Compare both results to values from experiments and comment on the differences.

2. Using an 8-atom cubic cell, 5^3 k-point sampling, and default energy cutoff, calculate the cohesive energy, equilibrium lattice dimensions and bulk modulus for Si. Then, remove one atom and calculate the formation energy of a Si vacancy (use bulk Si as reference). Assuming a formation entropy of 10k, estimate the resulting equilibrium concentration. Using nudged elastic band (NEB) method, calculate the vacancy migration energy and estimate the vacancy diffusivity assuming an attempt frequency of $10^{-13}s^{-1}$. From the density of states comment on the effect of changes in Fermi level on the equilibrium V concentration and diffusivity. (Note that 8 atom supercell is too small for accurate calculations of V properties, but provides a fast-running example.)

Extra credit: By calculating vibration frequencies, estimate the entropy of formation for a vacancy and the HTST attempt frequency.

3. Calculate something of interest to you. Please send your plan to me for comments/approval by Monday 10/27/13.