PHY801: Survey of Atomic and Condensed Matter Physics
Michigan State University

Homework 9

9.1. This problem on the cohesive energy of bcc and fcc neon compares the subtle difference between different types of crystal structures for Lennard-Jones solids and is based on Kittel Chapter 3, Problem #2. Using the Lennard-Jones potential, calculate the ratio of the cohesive energies of neon in the bcc and fcc structures. The lattice sums are

$$C_{12}(bcc) = \sum_j{}' p_j^{-12} = 9.11418 \; ; \;\; C_6(bcc) = \sum_j{}' p_j^{-6} = 12.2533$$

for the bcc lattice and

$$C_{12}(fcc) = \sum_j{}' p_j^{-12} = 12.13188 \; ; \;\; C_6(fcc) = \sum_j{}' p_j^{-6} = 14.45392$$

for the fcc lattice.

9.2. This problem on solid molecular hydrogen is based on Kittel Chapter 3, Problem #3. For H_2 one finds from measurements on the gas that the Lennard-Jones parameters are $\epsilon = 50\times10^{-16}$ erg and $\sigma = 2.96$ Å. Find the cohesive energy in kJ per mole of H_2; do the calculation for an fcc structure. Treat each H_2 molecule as a sphere. The observed value of the cohesive energy is 0.751 kJ/mol, much less than what you get, so that quantum corrections must be very important.

9.3. This problem involving the Madelung energy and repulsive energy for a linear ionic crystal is based on Kittel Chapter 3, Problem #5. Consider a line of $2N$ ions of alternating charge $\pm q$ with a repulsive potential energy A/R^n between nearest neighbors.

(a) Show that, in *cgs* units, at the equilibrium separation

$$U(R_0) = -\frac{2Nq^2 \ln 2}{R_0}\left(1 - \frac{1}{n}\right) \; .$$

(b) Let the crystal be compressed so that $R_0 \to R_0(1-\delta)$. Show that the work done in compressing a unit length of the crystal has the leading term $\frac{1}{2}C\delta^2$, where, in *cgs* units,

$$C = \frac{(n-1)q^2 \ln 2}{R_0} \; .$$

To obtain the results in SI, replace q^2 by $q^2/4\pi\epsilon_0$. Note: Do not expect to obtain this result from the expression for $U(R_0)$; you must use the complete expression for $U(R)$.

9.4. This problem about ionic crystals and their most stable ionic configuration is based on Kittel Chapter 3, Problem #7. Barium oxide has the NaCl structure. Estimate the cohesive energies per molecule of the hypothetical crystals Ba^+O^- and $Ba^{++}O^{--}$ with respect to separated neutral atoms. The observed nearest-neighbor internuclear distance is $R_0 = 2.76$ Å. The first and second ionization potentials of Ba are 5.19 eV and 9.96 eV, respectively. The electron affinities of the first and second electrons added to the neutral oxygen atom are 1.5 eV and -9.0 eV, respectively. The first electron affinity of the neutral oxygen atom is the energy released in the reaction $O + e \to O^-$. The second electron affinity is the energy released in the reaction $O^- + e \to O^{--}$. Which valence state do you predict will occur? Assume R_0 is the same for both forms, and neglect the repulsive energy.
