University of Alabama
Department of Physics and Astronomy

PH 253 / LeClair | Spring 2010

Problem Set 9

Instructions:

1. Answer all questions below. Show your work for full credit.
2. All problems are due Fri 2 Apr 2010 by the end of the day.
3. You may collaborate, but everyone must turn in their own work.

1. *Hydrogen-like systems.* Assuming a ^{3}Li atom to be hydrogen-like, determine the ionization energy of the $2s$ electron. Explain qualitatively the difference from the experimental value of 5.39 eV. *Hint: two approximations are to: a) neglect the inner electrons, or b) presume they shield the nucleus. These approximations bound the correct answer.*

2. *Energetics of diatomic systems I.* The dissociation energy of KI is 3.33 eV. Calculate the bond length (interionic distance) for KI given that the electron affinity of I is 3.06 eV and the ionization energy of K is 4.34 eV. (The measured bond length is 0.323 nm.) *Hint: the dissociation energy is the sum of the electrostatic energy required to separate the two species and the electron affinity, minus the ionization energy.*

3. *Energetics of diatomic systems II.* An approximate expression for the potential energy of two ions as a function of their separation is

$$\mathsf{PE} = -\frac{ke^2}{r} + \frac{b}{r^9} \tag{1}$$

The first term is the usual Coulomb interaction, while the second term is introduced to account for the repulsive effect of the two ions at small distances. **(a)** Find b as a function of the equilibrium spacing r_o. **(b)** Calculate the potential energy of KCl at its equilibrium spacing ($r_o = 0.279$ nm).

4. *Energetics of diatomic systems III.* An expression for the potential energy of two neutral atoms as a function of their separation r is given by the *Morse potential*,

$$\mathsf{PE} = P_o\left[1 - e^{-a(r-r_o)}\right]^2 \tag{2}$$

(a) Show that r_o is the atomic spacing and P_o the dissociation energy. **(b)** Calculate the force constant for small oscillations about $r = r_o$.

5. *Energetics of diatomic systems IV.* In the potassium iodide molecule, assume that the K and I atoms bond ionically by the transfer of one electron from K to I. **(a)** The ionization energy of K is 4.34 eV, and the electron affinity of I is 3.06 eV. What energy is needed to transfer an electron from K to I, to form K^+ and I^- ions from neutral atoms? This is sometimes called the activation energy E_a. **(b)** Another model potential energy function for the KI molecule is the Lennard-Jones potential:

$$U(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] + E_a \tag{3}$$

where r is the internuclear separation distance, and σ and ϵ are adjustable parameters. The E_a term is added to ensure correct asymptotic behavior at large r. At the equilibrium separation distance $r = r_o = 0.305\,\text{nm}$, $U(r)$ is a minimum, and $U(r_o) = -3.37\,\text{eV}$ is the negative of the dissociation energy. Evaluate σ and ϵ. **(c)** Calculate the force needed to break up a KI molecule. **(d)** Calculate the force constant for small oscillations about $r = r_o$. *Hint: Set* $r = r_o + \delta$, *where* $\delta/r_o \ll 1$ *and expand* $U(r)$ *in powers of* δ/r_o *up to second-order terms.*

6. *Crystal lattice energy.* Consider a one-dimensional chain of alternating positive and negative ions. Show that the potential energy associated with one of the ions and its interactions with the rest of this hypothetical crystal is

$$U(r) = -k_e \alpha \frac{e^2}{r} \tag{4}$$

where the Madelung constant is $\alpha = 2\ln 2$ and r is the interionic spacing. *Hint: the series expansion for* $\ln(1+x)$ *may prove useful in evaluating an infinite sum.*

7. *Free-electron gas I.* **(a)** Obtain an expression for the Fermi energy at $T = 0\,\text{K}$ for an electron gas in a metal in terms of the total number of electrons, the volume, and fundamental constants. **(b)** At $T = 0\,\text{K}$, what is the rms speed, in terms of the Fermi energy, of an electron gas in a metal?

8. *Free-electron gas II.* Show that the average kinetic energy of a conduction electron in a metal at 0 K is $E_{av} = \frac{3}{5} E_F$. *Hint: in general, the average kinetic energy is*

$$E_{av} = \frac{1}{n_e} \int E\, N(E)\, dE \tag{5}$$

where n_e is the density of particles, $N(E)\,dE$ is the number of electrons per unit volume that have energies in $[E, E + dE]$, and the integral is over all possible values of energy.

9. *Ohmic conduction.* An aluminum wire with a cross-sectional area of $4.00 \times 10^{-6}\,\text{m}^2$ carries a current of 5.00 A. Find the drift speed of the electrons in the wire. The density of aluminum is

$2.70\,\mathrm{g/cm^3}$; assume each Al atom provides a single electron for conduction. *Hint: how many atoms per unit volume are there? Use your periodic table.*