3. What type of bonding would be expected for each of the following materials:

a. Solid Xenon Van der Waals (secondary), since Xe is an inert gas

b. Calcium fluoride (CaF_2) predominantly ionic, since Ca will donate 2 electrons to F

c. Tungsten? metallic, since it is a single element with an unfilled shell.

^{20}Ca : [Ar] $4s^2$ ← has 2 extra e^-

^{9}F : [He] $2s^2 2p^5$ ← needs 1 e^- to fill the n=2 shell

4. Problem 1.7, parts (a) and (b) only.

(a) $E(r) = -2\varepsilon\left[14.45\left(\frac{\sigma}{r}\right)^6 - 12.13\left(\frac{\sigma}{r}\right)^{12}\right]$ eV/atom

$$\frac{dE}{dr} = -2\varepsilon\left[14.45\times(-6)\frac{\sigma^6}{r^7} - 12.13\times(-12)\frac{\sigma^{12}}{r^{13}}\right] =$$

$$= 2\varepsilon\left[86.7\frac{\sigma^6}{r^7} - 145.6\frac{\sigma^{12}}{r^{13}}\right] = 0$$

multiply by r^{13}:

$$2\varepsilon\left[86.7\sigma^6 r^6 - 145.6\sigma^{12}\right] = 0$$

$$r_0 = \left(\frac{145.6\sigma^{12}}{86.7\sigma^6}\right)^{1/6} = (1.679)^{1/6}\sigma = \boxed{1.090\sigma = r_0}$$

in Ne:

$\sigma = 0.274$ nm

$r_0 = 1.090\sigma = 0.299$ nm

(b) $$E(r_0) = -2(3.121\times10^{-3}\,\text{eV})\left[14.45\left(\frac{\cancel{\sigma}}{1.090\cancel{\sigma}}\right)^6 - 12.13\left(\frac{\cancel{\sigma}}{1.090\cancel{\sigma}}\right)^{12}\right] =$$

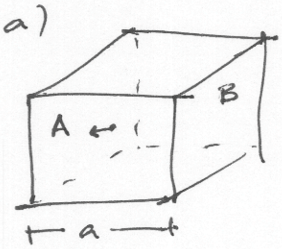
$= 0.027$ eV/atom

Derivation for Exam #1 Please be sure to show all of your work, with comments where necessary to make your derivation easy to follow. Try not to use your notes from class or the book (but if you get stuck, it might help you to read over Kasap section 1.4.1).

a) By considering a gas in a cubic container, derive an expression that relates the pressure (P), volume (V), and number of molecules (N) to the average kinetic energy per molecule ($\frac{1}{2}m\overline{v^2}$).

b) By comparing the expression above to the empirical gas equation $PV = \frac{N}{N_A}RT$ obtain a relationship between the average kinetic energy per molecule and temperature (T).

a)



When a molecule collides with face A, the change in momentum is in the x-direction only for a perfectly ellastic collision:

$$\Delta p = p_f - p_i = mv_x - (-mv_x) = 2mv_x$$

the molecule then goes to face B and comes back to A, the time interval between collisions is $\Delta t = \frac{2a}{v_x}$

and the force on wall A is

$$F = \frac{\Delta p}{\Delta t} = \frac{2mv_x}{2a/v_x} = \frac{mv_x^2}{a}$$

the total pressure of N molecules on face A is

$$P = \frac{F_{total}}{a^2} = \frac{mv_{x_1}^2 + mv_{x_2}^2 + \dots + mv_{x_N}^2}{a^3} = \frac{mN}{a^3} \cdot \frac{v_{x_1}^2 + v_{x_2}^2 + \dots + v_{x_N}^2}{N} = \frac{mN}{a^3}\overline{v_x^2}$$

since the molecules are in random motion,

$$\overline{v_x^2} = \overline{v_y^2} = \overline{v_z^2} \quad \text{and} \quad \overline{v^2} = \overline{v_x^2} + \overline{v_y^2} + \overline{v_z^2} = 3\overline{v_x^2}$$

then $P = \frac{mN}{a^3} \cdot \frac{1}{3}\overline{v^2} = \frac{Nm\overline{v^2}}{V} \rightarrow \boxed{PV = \frac{2}{3}N\left(\frac{1}{2}m\overline{v^2}\right)}$

b) $PV = \frac{N}{N_A}RT = NkT = \frac{2}{3}N\left(\frac{1}{2}m\overline{v^2}\right) \rightarrow \boxed{\overline{KE} = \frac{1}{2}m\overline{v^2} = \frac{3}{2}kT}$