NPRE 330 Hw 1

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1 Atomic Structure

1.1

The electronegativity of Li is 1.0 and the electronegativity of F is 4.0, which is the highest on the periodic table.

1.2

This would be an ionic bond as LiF is between a metal and a halogen and the difference in electronegativities is very high.

1.3

We know the equilibrium position occurs when the energy is minimized, which is when the derivative is zero. We know the derivative cannot have a maximum because maximum energy is non-physical.

$$E_{net} = E_A + E_R = -\frac{1.527}{r} + \frac{6.121e-6}{r^8} \tag{1}$$

$$\frac{d(E_{net})}{dr} = -1.527(-r^2) + 6.121e-6(-8r^{-9}) = 0 \tag{2}$$

$$\frac{1.527}{r^2} = \frac{4.8968e-5}{r^9} \tag{3}$$

$$r_{eq} = \left(\frac{4.8968e-6}{1.527}\right)^{\frac{1}{7}} = 0.22804\ nm \tag{4}$$

Plugging the equilibrium radius into Eq. 1, we obtain the equilibrium energy.

$$E_{eq} = -5.85918\ eV \tag{5}$$

1.4

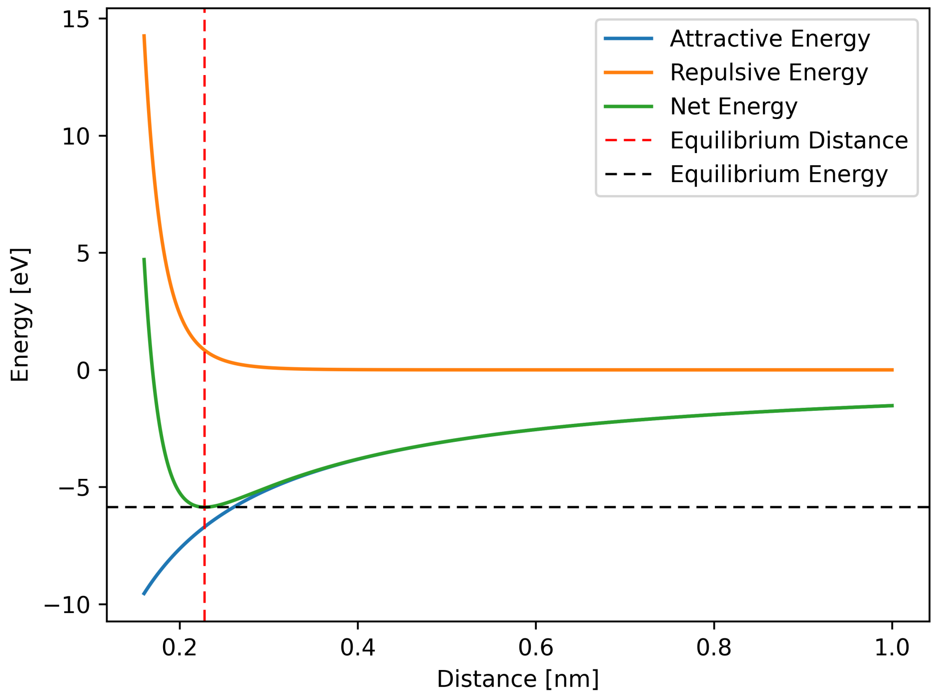

Figure 1: Plot of Energies against Radius

2 Atomic Structure

2.1

The force of attraction is given in Callister in Eq 2.5b:

$$F_a = \frac{dE_a}{dr} \tag{6}$$

And E_a is given in Eq 2.9 as:

$$E_a = \frac{-A}{r} \tag{7}$$

Combining these two equations:

$$F_a = \frac{d\left(\frac{-A}{r}\right)}{dr} = \frac{A}{r^2} \tag{8}$$

With Eq 2.10, A is given as:

$$A = \frac{e^2|Z_1||Z_2|}{4\pi\epsilon_0} \tag{9}$$

Combining Eq. 8 and Eq. 9:

$$F_a = \frac{e^2|Z_1||Z_2|}{4\pi\epsilon_0 r^2} \tag{10}$$

Solving for r:

$$r = r_{Mg^{2+}} + r_{F^-} = 0.072nm + 0.133nm = 0.205nm = 0.205e-9m \tag{11}$$

Substituting the values for e, ϵ_0, and r:

$$F_a = \frac{(2.31e-28N \cdot m^2)|Z_{Mg^{2+}}||Z_{F^-}|}{(0.205e-9m)^2} \tag{12}$$

With $|Z_{Mg^{2+}}| = 2$ and $|Z_{F^-}| = 1$, we get the final answer:

$$F_a = 1.09935e-08\ N \tag{13}$$

2.2

Operating under the assumption that the interionic separation distance is the equilibrium distance:

$$F_r = -F_a = -1.09935e-08\ N \tag{14}$$

3 Crystal Lattices

3.1

An HCP unit cell is a hexagonal prism with a top face that is a hexagon. This hexagon can be broken into 6 equilateral triangles with side lengths a. Therefore, the area of the top face is given as:

$$A = 6 * a_t = 6\left(\frac{\sqrt{3}a^2}{4}\right) = \frac{3a^2c\sqrt{3}}{2} \tag{15}$$

The area of the top face is then multiplied by the height of the prism c:

$$V = c \cdot A = \frac{3a^2c\sqrt{3}}{2} \tag{16}$$

We know at $a = 2R$ where R is the atomic radius. We also know $\frac{c}{a} = 1.568 \therefore c = 1.568a$. With this, the volume can be written purely in terms of the atomic radius.

$$V = \frac{3(1.568)a^3\sqrt{3}}{2} = \frac{4.704(2R)^3\sqrt{3}}{2} = 18.816\sqrt{3}R^3 = 32.590R^3 \tag{17}$$

Knowing that the radius of Be is $0.1143e-9m$:

$$V = 32.590(0.1143e-9\ m)^3 = 4.867e-29\ m^3 = 0.04867\ nm^3 \tag{18}$$

3.2

To calculate the theoretical density of Be, we can use Eq. 3.8 from Callister.

$$\rho = \frac{nA}{VN_A} \tag{19}$$

Where n is the number of atoms in the unit cell, A is the atomic weight, V is the volume of the unit cell, and N_A is Avogadro's number.

Substituting the values for this problem:

$$\rho = \frac{(6)(9.0121831\ g/mol)}{(4.867e-29\ m^3)(6.022e23\ atoms/mol)} = 1.845e6\ g/m^3 = 1.845\ g/cc \tag{20}$$

The theoretical density of 1.845 g/cc agrees very closely with the experimental density of 1.848 g/cc.

4 Crystal Lattices

To find the radius of Pd knowing we have and FCC structure, density of 12.0 g/cc, and an atomic weight of 106.4 g/mol, we can use Eq. 19.

$$\rho = \frac{nA}{VN_A} \longrightarrow V = \frac{nA}{\rho N_A} \tag{21}$$

We know all the values on the right side of the equation, so only need to find the volume of an FCC unit cell. We know the diagonal of the unit cell is $4R$, so we can say that each side length is given as follows:

$$a^2 + a^2 = (4R)^2 \longrightarrow a = 2R\sqrt{2} \tag{22}$$

We also know that the volume of the cell is a^3, so volume is given as follows:

$$V = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2} \tag{23}$$

Substituting the formula for volume in terms of radius into Eq. 21, we obtain the formula for radius.

$$16R^3\sqrt{2} = \frac{nA}{\rho N_A} \tag{24}$$

$$R^3 = \frac{\sqrt{2}nA}{32\rho N_A} \tag{25}$$

$$R = \left(\frac{\sqrt{2}nA}{32\rho N_A}\right)^(1/3) \tag{26}$$

$$R = \left(\frac{\sqrt{2}(4\ atoms)(106.4\ g/mol)}{32(12\ g/cm^3)(6.022e23\ atoms/mol)}\right)^{1/3} = 1.376e7\ cm = 0.1376\ nm \tag{27}$$

This is very close agreement with the 0.137 nm given online.