Problem 1

(a) 8
(b) \(6(1/2) + 8(1/8) = 3 + 1 = 4\)
(c) 4
(d) 8
(e) F cubic Bravais lattice
(f) 2 \(\text{Na}^+\) and 1 \(\text{O}^{2-}\) in the basis
(g) \(\text{Na}^+\) and \(\text{O}^{2-}\) touch each other along the body diagonal of the cube. Thus,
\[
r + R = \frac{\sqrt{3}}{4} a
\]
(h) Density = \(\frac{\text{Mass of unit cell}}{\text{Volume of unit cell}}\)

Mass of unit cell = 4 (16 amu) + 8 (23 amu)
\[
= 248 \text{ amu}
\]
\[
= 248 \text{ amu} \times \frac{1}{6.02 \times 10^{23} \text{ amu/g}}
\]
\[
= 4.12 \times 10^{-22} \text{ g}
\]

From the periodic table,
\[
r = 0.95 \, \text{Å}
\]
\[
R = 1.40 \, \text{Å}
\]

Hence, according to the result of (g),
\[
a = 4 \left( \frac{r + R}{\sqrt{3}} \right) = 5.427 \, \text{Å}
\]

Volume of unit cell = \(a^3 = (5.427 \, \text{Å})^3 = 1.598 \times 10^2 \, \text{Å}^3 = 1.598 \times 10^{-22} \, \text{cm}^3\)

Density = \(\frac{4.12 \times 10^{-22} \text{ g}}{1.598 \times 10^{-22} \, \text{cm}^3} = 2.58 \, \text{g/cm}^3\)
Problem 2

(a) 1

(b) \(6 \times (1/3) + 1 = 2 + 1 = 3\)

(c) parallelogram

(d)

(e) 3

(f)

\[a = \frac{4r}{\sqrt{2}}\]

Problem 3

For FCC,

For lead, \(r = 1.750 \text{ Å}\),

Thus

\[a = \frac{4}{\sqrt{2}} (1.750 \text{ Å})\]

\[= 4.950 \text{ Å}\]
Volume of the unit cell = \( a^3 \)
= \((4.950 \, \text{Å})^3\)
= \(121 \, \text{Å}^3\)

Problem 4

For the HCP structure,

\[ a = 2r. \]

For Mg, \( r = 1.61 \, \text{Å} \) (given).

Thus, \( a = 2 \times (1.61 \, \text{Å}) = 3.22 \, \text{Å} \)

Since \( \frac{c}{a} = 1.62 \),

\( c = 1.62 \times a = 1.62 \times (3.22 \, \text{Å}) = 5.21 \, \text{Å} \).

Consider the hexagonal unit cell of the HCP structure.
No. of atoms per unit cell = 6

Volume of a unit cell = \( \frac{3}{2} \sqrt{3} \, a^2 \, c \)

Density = \( \frac{\text{Mass of atoms in a unit cell}}{\text{Volume of a unit cell}} \)

\[ = \frac{6 \left( \frac{24.31 \, \text{g}}{6.02 \times 10^{23}} \right)}{2 \sqrt{3} \, (3.22 \, \text{Å})^2 \, (5.21 \, \text{Å})} \]

= 1.73 \, \text{g/cm}^3

Problem 5

The electron energy levels for a copper atom are \( E_K = -8982 \, \text{eV}, E_L = -933 \, \text{eV}, \) and \( E_M = -75 \, \text{eV}. \) Calculate (a) the \( K\alpha \) photon energy, (b) the \( K\beta \) photon energy, (c) the \( L\alpha \) photon energy, (d) the \( KLL \) Auger electron energy, and (e) the \( LMM \) Auger electron energy.

(a) \( E_{K\alpha} = |E_K - E_L| = |-8982 \, \text{eV} - (-933 \, \text{eV})| = 8049 \, \text{eV} \)

(b) \( E_{K\beta} = |E_K - E_M| = |-8982 \, \text{eV} - (-75 \, \text{eV})| = 8907 \, \text{eV} \)

(c) \( E_{L\alpha} = |E_L - E_M| = |-933 \, \text{eV} - (-75 \, \text{eV})| = 858 \, \text{eV} \)

(d) \( E_{KLL} = |E_K - E_L - |E_L| = 8049 \, \text{eV} - 933 \, \text{eV} = 7116 \, \text{eV} \)

(e) \( E_{LMM} = |E_L - E_M - |E_M| = 858 \, \text{eV} - 75 \, \text{eV} = 783 \, \text{eV} \)
Problem 6

The K shell electron energy for nickel is \( E_K = -8333 \text{ eV} \) and the wavelengths of the NiK\(_α\) and NiK\(_β\) photons are 0.1660 nm and 0.1500 nm, respectively. (a) Draw an energy-level diagram for a nickel atom. Calculate (b) the KLL and (c) the LMM Auger electron energies for nickel.

(a) \( |E_K - E_L| = E_{KL} = \frac{hc}{\lambda_{K\alpha}} \)

\[
= \frac{0.6626 \times 10^{-33} \text{ J s}}{(0.2998 \times 10^9 \text{ m/s})} \frac{(0.1660 \times 10^{-9} \text{ m})(1 \text{ J} / 6.626 \times 10^{-34} \text{ J s})}{(0.1500 \times 10^{-9} \text{ m})(1 \text{ J} / 6.626 \times 10^{-34} \text{ J s})}
\]

= 7470 eV

\( \therefore E_L = -8333 \text{ eV} + 7470 \text{ eV} = -863 \text{ eV} \)

\( |E_K - E_M| = E_{K\beta} = \frac{hc}{\lambda_{K\beta}} \)

\[
= \frac{0.6626 \times 10^{-33} \text{ J s}}{(0.2998 \times 10^9 \text{ m/s})} \frac{(0.1500 \times 10^{-9} \text{ m})(1 \text{ J} / 6.626 \times 10^{-34} \text{ J s})}{(0.1500 \times 10^{-9} \text{ m})(1 \text{ J} / 6.626 \times 10^{-34} \text{ J s})}
\]

= 8266 eV

\( \therefore E_M = -8333 \text{ eV} + 8266 \text{ eV} = -67 \text{ eV} \)

Given the diagram:

\[ -863 \text{ eV} \]

\[ -8333 \text{ eV} \]

\[ 0 \text{ eV} \]

\[ -67 \text{ eV} \]

\[ \uparrow \]


(b) \( E_{KLL} = |E_K - E_L| - |E_M| \)

= 7470 eV - (863 eV) = 6607 eV

(c) \( E_{LMM} = |E_L - E_M| - |E_M| \)

= \( | -863 \text{ eV} - (-67 \text{ eV})| - | -67 \text{ eV}| \)

= 796 eV - 67 eV = 729 eV