

# Exam 1

Thursday, September 30, 2021 3:35 PM

## Question 12

B.1 (a) Calculate the % ionic character in a compound  $AB_2$  if the electronegativities of Y and X are 0.7 and 3 respectively.

(b) On the basis of the result in (a), what type(s) of interatomic bonding would you expect to be dominant in  $AB_2$ ?

$$a.) \% \text{ IC} = \left( 1 - e^{\left( -\frac{(\chi_Y - \chi_X)^2}{4} \right)} \right) \times 100$$

$$\% \text{ IC} = \left( 1 - e^{\left( -\frac{(0.7 - 3)^2}{4} \right)} \right) \times 100$$

$$\% \text{ IC} = 73.35\%$$

b.)

Mainly ionic bonds

## Question 13

10 pts

Part B.2: If the energy of attraction between a divalent anion and a monovalent cation is  $-1.7 \times 10^{-18}$  J, calculate their internuclear distance of separation (in nm).

$$F(r) = \frac{|z_1 z_2| e^2}{4 \pi \epsilon_0 r^2}$$

$$-1.7 \times 10^{-18} = \frac{2 (1.602 \times 10^{-19})^2}{4 \pi (8.85 \times 10^{-12}) r^2}$$

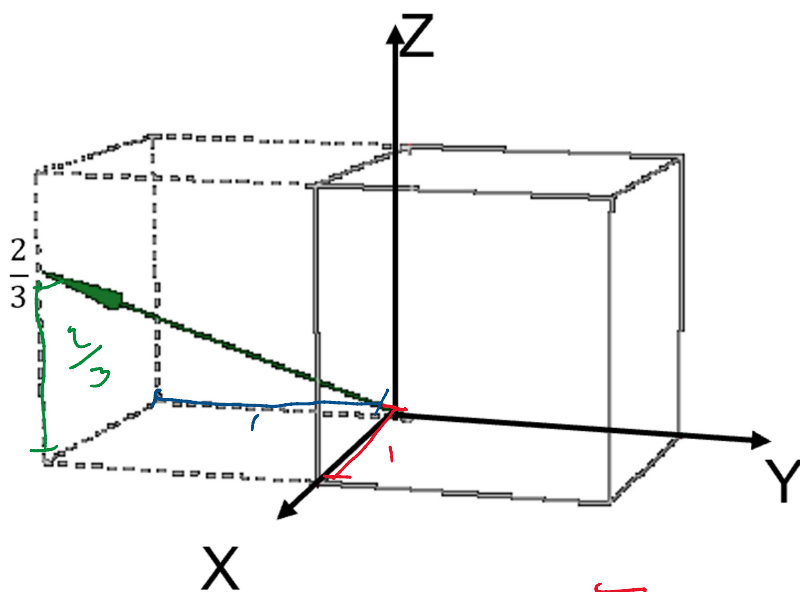
$$J = \frac{N}{m}$$

$$1.891 \times 10^{-28} = \frac{5.183 \times 10^{-38}}{r^2}$$

$$r = \sqrt{\frac{5.183 \times 10^{-38}}{1.891 \times 10^{-28}}} = 1.647 \times 10^{-5} = 16470 \text{ nm}$$

# Question 14

Part B.3: Determine the direction's indices in the cubic unit cell below

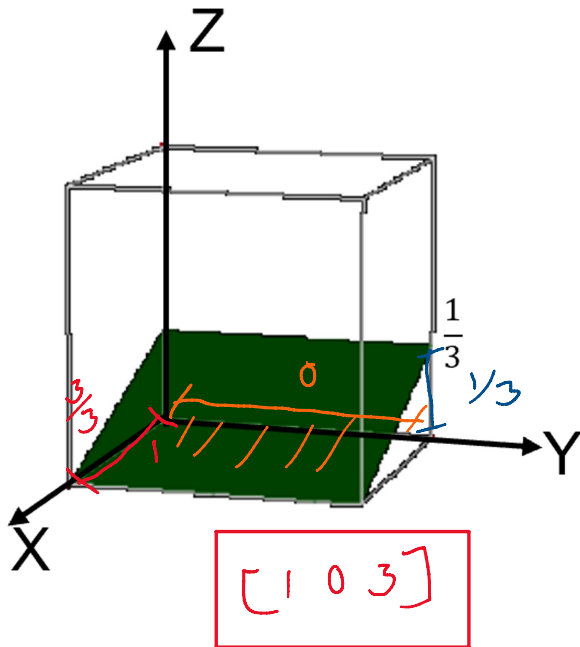


$$3 \left[ \left( 1, -1, \frac{2}{3} \right) \right]$$

$$= [3 \bar{3} 2]$$

### Question 15

Part B.4: Determine the plane's indices in the cubic unit cell below.



$$\begin{aligned} \frac{1}{\frac{1}{3}} - 0 &= 3 \\ 0 - 0 &= 0 \\ \frac{3}{1} - 0 &= 3 \end{aligned}$$

### Question 16

10 pts

Part B.5: Determine the theoretical density of a hypothetical metal having a BCC crystal structure [in  $\text{g/cm}^3$ ] if the metal has an atomic radius of 0.19 nm and an atomic weight of 100.5 g/mol.

$$\rho = \frac{nA}{V_c N_A}$$

$$\rho = \frac{(2)(100.5)}{(8.498 \times 10^{-23})(6.022 \times 10^{23})}$$

$$\rho = 3.95 \text{ g/cm}^3$$

$$V_c = \left( \frac{4R}{\sqrt{3}} \right)^3$$

$$V_c = \left( \frac{(1.9 \times 10^{-8})(4)}{\sqrt{3}} \right)^3$$

$$V_c = 8.498 \times 10^{-23}$$

## Question 17

10 pts

Part B.6: A pure FCC metal sample was analyzed with an X-ray beam of wavelength 0.075 nm and the observed diffraction angle for the first-order reflection from the (211) set of planes was 27.1°. Calculate the atomic radius of the metal and identify the metal

$$d = \frac{n\lambda}{2\sin(\theta)}$$

$$d = \frac{(1)(0.075 \times 10^{-9})}{2\sin(27.1^\circ)} = 8.23 \times 10^{-11}$$

$$a = \frac{4R}{\sqrt{2}} = d\sqrt{(h)^2 + (k)^2 + (l)^2}$$

$$\frac{4R}{\sqrt{2}} = (8.23 \times 10^{-11})\sqrt{6}$$

$$R = 7.13 \times 10^{-11} \text{ m} = \boxed{0.0713 \text{ nm}}$$

The metal is  $\text{Mg}^{2+}$

## Question 18

10 pts

Part B.7: Calculate the temperature [in K] required to increase the fraction of vacancies in a metal from  $0.5 \times 10^{-5}$  to  $1.5 \times 10^{-5}$ , if the energy of vacancy formation is 2.1 eV/atom.

$$\frac{N_v}{N} = \exp\left(\frac{-Q_v}{k_B T}\right)$$

$$\frac{1.5 \times 10^{-5}}{0.5 \times 10^{-5}} = \exp\left(\frac{-2.1}{(8.617 \times 10^{-5} \text{ T})}\right)$$

$$\ln(3) = -\frac{2.1}{k_B T}$$

$$T = 22182.92 \text{ K}$$