1 Module 2

The Coloumbic Force:

$$F_C = \frac{-k_0(Z_1 q)(Z_2 q)}{a^2}$$

Where:

1. Z is the valence of the charge ion
2. q is electron charge ($0.16 \times 10^{-18} C$)
3. k_0 is proportionality ($9 \times 10^9 V \cdot m \cdot C^{-1}$)
4. a is the distance between ion centres

The Repulsive Force:

$$F_R = \lambda e^{\frac{-a}{p}}$$

Where:

1. λ & p are given constants
2. a is the distance between ion centres

Coordination Number (CN):

CN	$\frac{r}{R}$ min	$\frac{r}{R}$ max
2	0	0.155
3	0.155	0.225
4	0.225	0.414
6	0.414	0.732
8	0.732	0.999
12	1	1

Bonding Energy:

$$E = \int_{\infty}^{a} F\,da = \int_{\infty}^{a} F_C\,da + \int_{\infty}^{a} F_R\,da$$

Percent Ionic Character:

$$\%IC = (1 - e^{-\frac{(X_A - X_B)^2}{4}}) \cdot 100\%$$

Reaction Enthalpy:

$$\Delta H_{rxn} = \sum BE_{reactants} + \sum BE_{products}$$

Thermal Expansion:

$$\frac{\Delta L}{L_0} = \alpha(T_2 - T_1)$$

Note: Temperature is in Kelvin

2 Module 3

Atomic Packing:

Atomic Packing Factor:

$$APF = \frac{V_{Atoms\ in\ unit\ cell}}{V_{Unit\ cell}}$$

Table of Common Packings:

Structure	CN	APV	APF
SC	6	1	$\frac{(1)(\frac{4}{3}\pi(\frac{a}{2})^3)}{a^3}; R = \frac{a}{2}$
BCC	8	2	$\frac{(2)(\frac{4}{3}\pi(\frac{\sqrt{3}a}{4})^3)}{a^3}; R = \frac{\sqrt{3}}{4}a; l = \sqrt{3}a$
FCC	12	4	$\frac{(4)(\frac{4}{3}\pi(\frac{\sqrt{2}a}{4})^3)}{a^3}; R = \frac{\sqrt{2}}{4}a$
HCP	12	2	$\frac{(2)(\frac{4}{3}\pi(\frac{a}{2})^3)}{Ac}; A = \frac{\sqrt{3}}{2}a^2; R = \frac{a}{2}; c = \sqrt{\frac{8}{3}}a$

Theoretical Density:

$$\rho = \frac{m_{Atoms\ in\ unit\ cell}}{V_{Unit\ cell}} = \frac{nA}{V_C N_A}$$

Where:

1. n is # atoms in unit cell
2. A is atomic weight
3. V_C is volume of unit cell
4. N_A is Avocado's number (6.022×10^{23})

Ionic Packing:

Ionic Packing Factor:

$$IPF = \frac{V_{ions}}{V_{Unit\ cell}}$$

Table of Common Packings:

Structure	CN	$\frac{r}{R}$ range
Simple Cubic (MX)	8	$[0.732, 1.0]$
Face Cent. Cubic (MX_2)	4/8	$[,]$

Theoretical Density:

$$\rho = \frac{m_{cell}}{V_{cell}} = \frac{\sum m_{Ci} + \sum m_{Aj}}{V_{cell}} = \frac{\sum n_{Ci} A_{Ci} + \sum n_{Aj} A_{Aj}}{V_{cell} N_A}$$

Where:

1. n is # of species in unit cell
2. A is atomic weight
3. V_C is volume of unit cell
4. N_A is Avocado's number (6.022×10^{23})

Semiconductors:

Table of Common Packings:

Structure	CN	Ions Per Cell
Diamond Cubic	4	8
Zinc Blende	4	4/4

Describing Crystal Structures:

Angle between Lattice Directions:

$$|\vec{u}| \cdot |\vec{v}| \cos(\theta) = \vec{u} \cdot \vec{v}$$

Determining Lattice Planes:

1. Read intercepts of plane in a, b, c
2. Take reciprocals, Reduce to integers

Bragg's Law:

$$n\lambda = 2d \sin\theta_{hkl}$$

Where:

1. θ Bragg's Angle = $\frac{1}{2}\times$ Diffraction Angle
2. d Interplanar Spacing
3. λ Radiation Wavelength
4. n order of reflection $n \in \mathbb{Z}$

D-Spacing (Cubic):

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Prediction of XRD patterns:

Table of Common pattern prediction:

Peak Order	h	k	l	$h^2+k^2+l^2$	SC	BCC	FCC
1	1	0	0	1	✓	×	×
2	1	1	0	2	✓	✓	×
3	1	1	1	3	✓	×	✓
4	2	0	0	4	✓	✓	✓
5	2	1	0	5	✓	×	×
6	2	1	1	6	✓	✓	×
7	2	2	0	8	✓	×	✓

SC: (100), (110), (111)
BCC: (110), (200), (211)
FCC: (111), (200), (220)