1 Module 2

The Coloumbic Force:

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

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

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	APF
Simple Cubic (SC)	6	1
Body Centered Cubic (BCC)	8	2
Face Centered Cubic (FCC)	12	4
Hexagonal Close-Packed (HCP)	12	6

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 Centered 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: