

# Structure of Solids

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**Exercises**  
**Descriptions of Simple Ionic**  
**Structures**

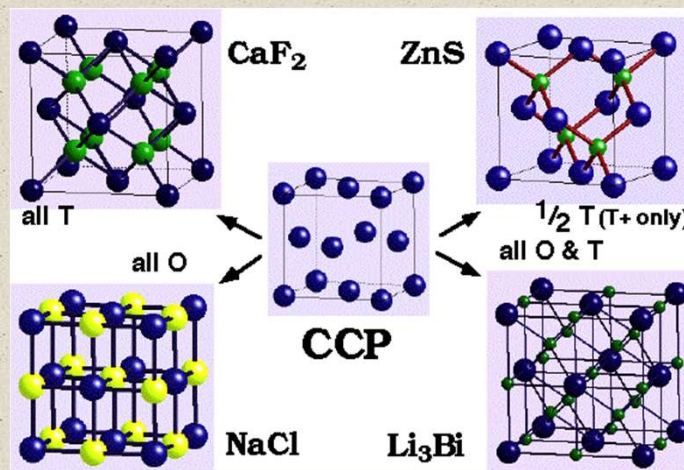
## How to describe the structure of an ionic solid?

1. Describe the structure as filling of interstitial holes in close-packing
2. Draw the unit cell in a plan or perspective view
3. Recognize the structure from a plan or perspective view of a unit cell
4. Identify coordination numbers & geometries of atoms
5. Give examples of adoption

3

## 1. Filling of interstitial holes in close-packing

- Ionic (and other) structures may be derived from the occupation of interstitial sites in close-packed arrangements



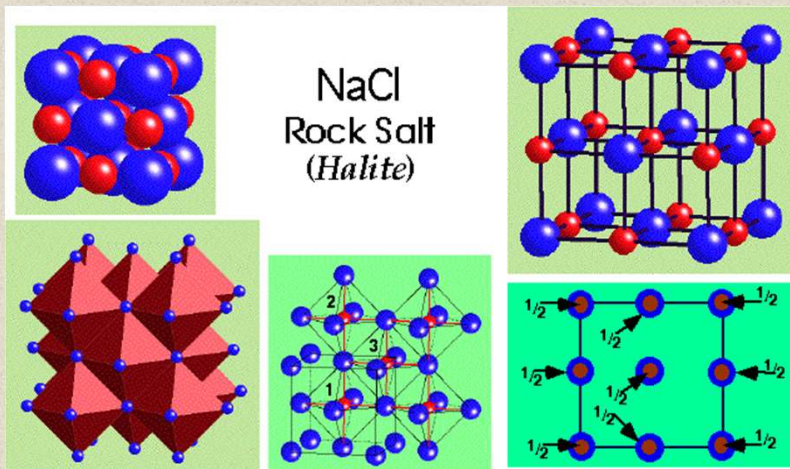
## Descriptions of some common structures

I. STRUCTURES DERIVED FROM CUBIC CLOSE PACKING (CCP)

II. STRUCTURES DERIVED FROM CUBIC CLOSE PACKING (CCP)

5

## NaCl Rock Salt



6

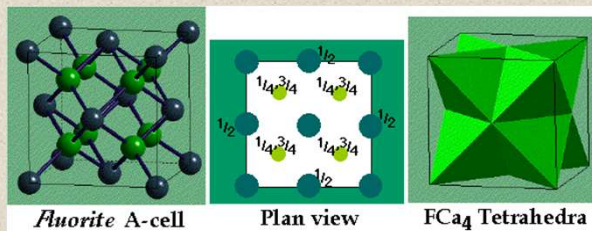


## NaCl Rock Salt

- AX compound
- c.c.p.  $\text{Cl}^-$  with  $\text{Na}^+$  in all Octahedral holes
- Lattice: fcc
- Motif: Cl at (0, 0, 0); Na at  $(\frac{1}{2}, 0, 0)$
- 4 NaCl in unit cell
- **Coordination: 6 : 6 (octahedral)**
- Cation and anion sites are topologically identical
- The fcc nature of the lattice can be seen by examining just one atom of the motif at a time (*i.e.* just  $\text{Cl}^-$  or just  $\text{Na}^+$ )

7

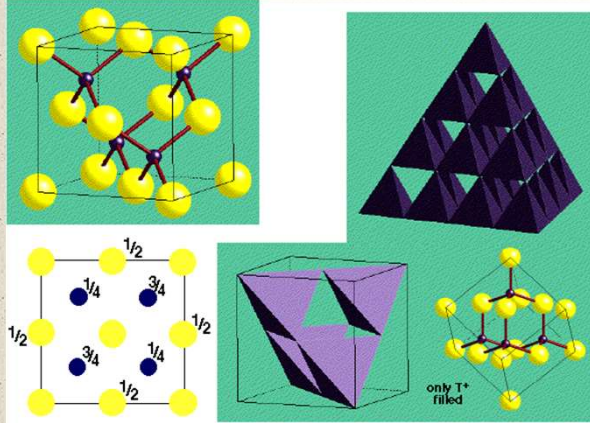
## $\text{CaF}_2$ Fluorite / $\{\text{Na}_2\text{O}$ Anti-Fluorite }



- $\text{AX}_2$  compound
- CCP  $\text{Ca}^{2+}$  with F in all Tetrahedral holes
- **Lattice: fcc**
- **Motif:  $\text{Ca}^{2+}$  at (0,0,0);  $2\text{F}^-$  at  $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$  &  $(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$**
- $4\text{CaF}_2$  in unit cell
- **Coordination:  $\text{Ca}^{2+}$  8 (cubic) : F 4 (tetrahedral)**
- In the related Anti-Fluorite structure Cation and Anion positions are reversed

8

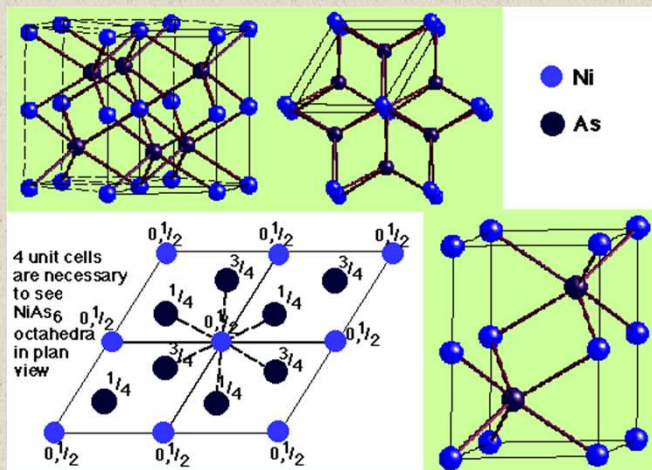
## ZnS Zinc Blende (Sphalerite)



AX, CCP  $S^{2-}$  with  $Zn^{2+}$  in half Tetrahedral holes (only  $T^+$  {or  $T^-$ } filled)  
 Lattice: fcc , 4ZnS in unit cell  
 Motif: S at (0,0,0); Zn at (1/4,1/4,1/4)  
 Coordination: 4:4 (tetrahedral)

9

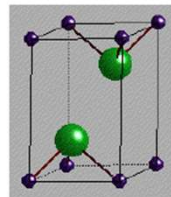
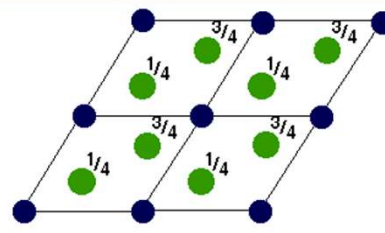
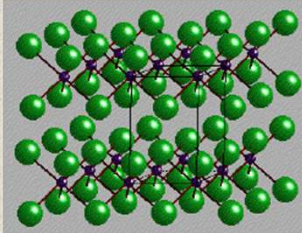
## NiAs Nickel Arsenide



HCP As with Ni in all Octahedral holes , Lattice: Hexagonal - P  
 $a = b, c = (8/3)a$   
 Motif 2Ni at (0,0,0) & (0,0,1/2) 2As at (2/3,1/3,1/4) & (1/3,2/3,3/4)  
 2NiAs in unit cell , Coordination: Ni 6 (octahedral) : As 6 (trigonal prismatic)

10

# CdI<sub>2</sub> Cadmium Iodide



Comparison

CdI<sub>2</sub>

vs

NiAs

