CH 411 Advanced Inorganic Chemistry, Fall 2018

CONCEPTS OUTLINE, WEEKS 1-5

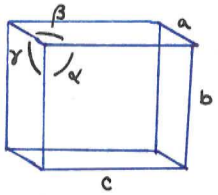
13 ∘ XI ∘ 18

There are seven types of

UNIT CELLS

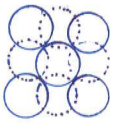
	$a \neq b \neq c$	$a = b \neq c$	$a = b = c$
$\alpha = \beta = \gamma$	ORTHO-RHOMBIC ◪	TETRA-GONAL ◪	CUBIC ◪ + TRIGONAL ($\frac{n}{3}$)
◪ $= \alpha = \beta \neq \gamma$	MONOCLINIC	HEXA-GONAL	∅
◪ $\neq \alpha \neq \beta \neq \gamma$	TRICLINIC	∅	∅

wherein



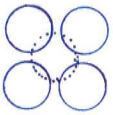
can exhibit

SIMPLE packing,



FACE-CENTERED packing, (a.k.a. xcp)

or



BODY-CENTERED packing.

The unit cells, in combination with various packing arrangements, yield the fourteen BRAVAIS LATTICE structures.

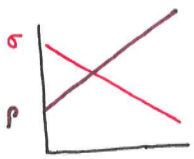
Ruling out thermodynamically unfavorable* configurations results in the CRYSTAL STRUCTURE TYPES:

(UNARY: Diamond (ZnS-esque) + Most metals.);

(BINARY: (1:2: CaF_2 Fluorite 50 cubic CN 4:8;
CdI_2 50 O_h-hcp CN 3:6;
$CdCl_2$ 50 O_h-ccp CN 3:6);
(1:1: (cubic (.733, 1) 71% anion radius: CsCl 100 cubic CN 8:8);
(O_h (.414, .732) ~41% a.r.: NiAs 100 hcp CN 6:6;
NaCl Rock Salt 100 ccp CN 6:6);
(T_d (.225, .414) ~22% a.r.: ZnS Wurtzite 50 hcp CN 4:4;
ZnS Zinc Blende 50 ccp CN 4:4));
(2:1: (T_d: [Does Not Exist] 100 hcp CN 8:4;
Antifluorite 100 ccp CN 8:4)));
(TERNARY: ABO_3 Perovskite B 25 O_h cubic;
AB_2O_4 Spinel B 50 O_h A 12.5 T_d ccp;
AB_2O_4 Spinel^{-1} B 25 O_h 12.5 T_d A 25 O_h ccp)

* via the Born-Mayer equation.

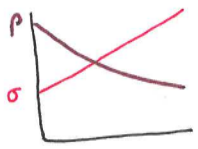
ELECTRICAL CONDUCTIVITY



INSULATORS

(4, +∞]-eV E_g; large Δx;
((>>20), (>7))-$(\Omega cm)^{-1}$ σ

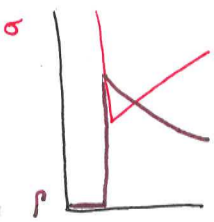
Empty conduction band w/all e⁻s in the valence band @ 0K.



SEMICONDUCTORS

[1, 4]-eV E_g; small Δx;
((>>7), (<<2))-$(\Omega cm)^{-1}$ σ

Can be either intrinsic/pure (e.g. GaAs) or extrinsic/doped (eg. SnO_2:F);
e⁻ behavior is quite diverse (see right).

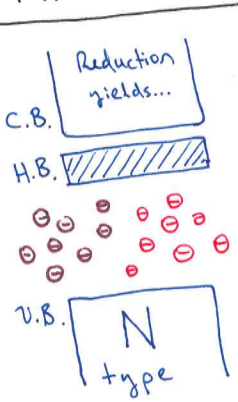


METALS

[0, 1)-eV E_g;
zero Δx;
(<<2, <<8)-$(\Omega cm)^{-1}$ σ
e⁻s spread btwn valence and conduction bands; 0ρ near 0K. (superconductivity)

N-TYPE vs. P-TYPE

a comparison of: semiconductors.



eg. Sn: In_2O_3
Si: P

eg. In: SnO_2
Si: Al

Some common E_gs in eV:

α-Sn	<0.1
Ge	0.66
Si	1.1
GaAs	1.42
ZnSe	2.7
CuBr	2.9
C	5.5

GOOD LUCK!!