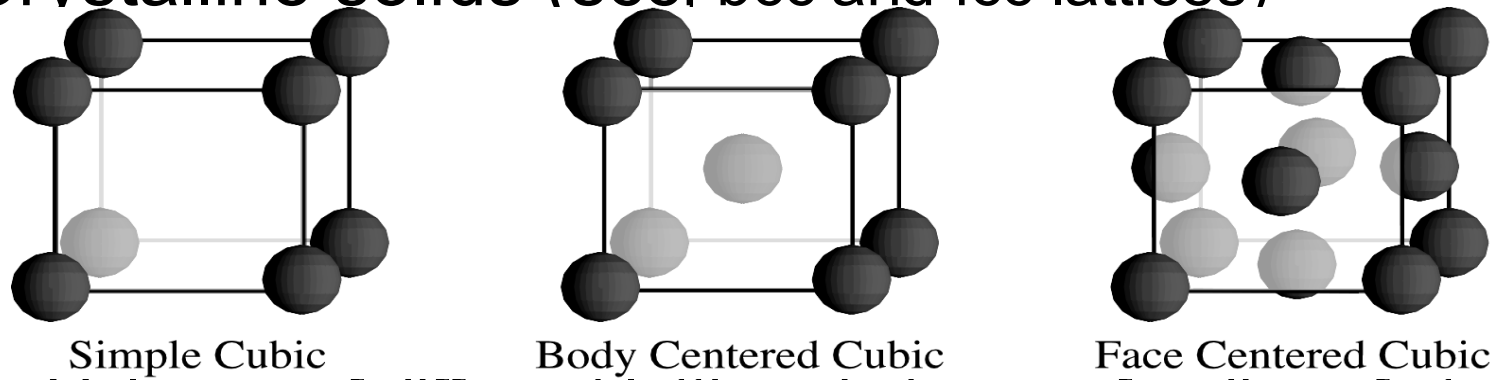
Announcements

- Last exam 1 week from Today.
- Lab does not meet the last week of the semester.

- Next week you will have an analytical reasoning quiz in discussion.

Review

- X-ray diffraction (small lattice spacing larger diffraction angles).
- Crystalline solids (scc, bcc and fcc lattices)



Simple Cubic | Body Centered Cubic | Face Centered Cubic

  - Volumes of different lattices in terms of radius of atoms:
- $V_{cubic} = 8r^3$, $V_{bcc} = \left(4/\sqrt{3}\right)^3 r^3$ $V_{fcc} = \left(16\sqrt{2}\right)r^3$
  - Calculated densities using this information.
  - Other things you can calculate (practice problems in text): Use density and unit cell size to get # of atoms per unit cell and ID type of unit cell. Unit cell type and density to get unit cell dimensions.

LiF (or NaCl)

Chang Figures 2.12 and 12.21

CsCl (interdigitated simple cubic)

Chang figure 12.20 a

Graphite

Chang Fig. 12.22 b

Buckminster Fullerene

Diamond

Chang Fig. 12.22 a

Metallic bonding (electron sea or jellium model)

Ion core of each metal atom is immersed in a sea of valence electrons that are delocalized over the whole crystal.

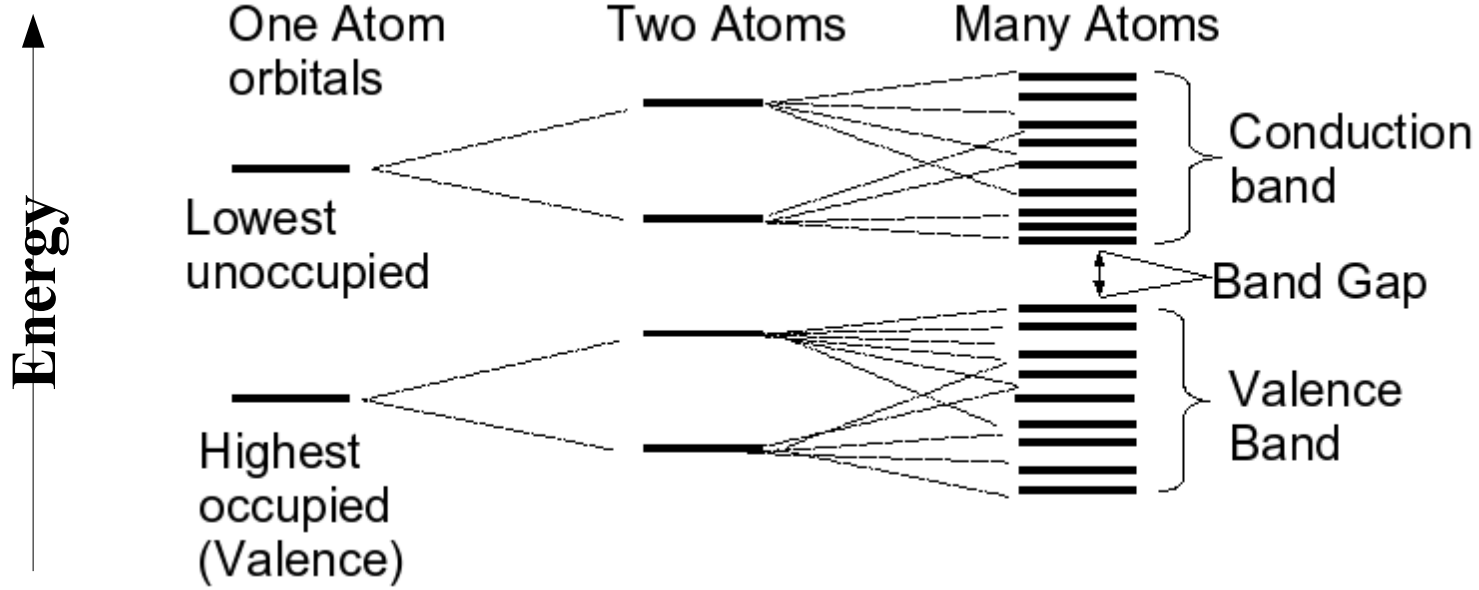
Chang Figure 12.23

Band Theory I (combining atomic orbitals on separate atoms)

Chang Figure 10.22

Key Idea: When two atomic orbitals on two different atoms are combined the two orbitals you get are different energies. One lower energy than the original orbitals one higher energy.

Band Theory II
(Combining lots of atoms/orbitals)



- Conduction band orbitals are delocalized over the whole solid.
- Valence band orbitals are localized to particular atoms or groups of atoms.
- There are only enough electrons to fill the valence band.
- Electrons need energy to jump across band gap to conduction band.

How Band Theory Explains Electrical Conductivity

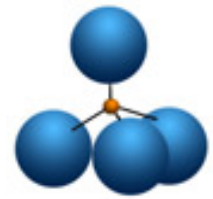
- Size of band gap dictates electrical properties.
  - Non-conductors (insulators) have large band gap. Thermal energy is not enough to promote electrons into conduction band.
  - Semi-conductors have a small band gap. Thermal energy is enough to promote some electrons into the conduction band.
  - Conductors (metals) have no band gap. Thus valence electrons are delocalized over whole system and can carry electricity.

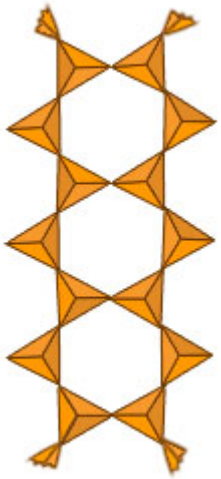
Synthetic Yellow Diamond

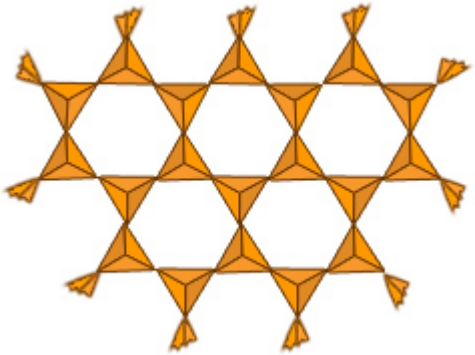
Picture from Feb. 2, 2004 *Chemical and Engineering News*

Band gap is sensitive to trace impurities (1 in 10^5 or even less). In this case trace amounts of N impurities decrease the band gap to the point where visible photons can excite the electrons.

Silicates







SiO_4^{4-} SiO_3^{2-} $Si_4O_{11}^{6-}$ $Si_2O_5^{2-}$

See Vision Learning Web Site (Minerals III) for better figures.