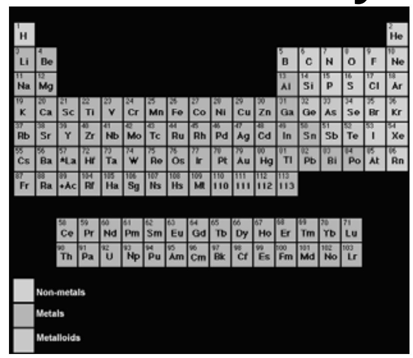
The Periodic Table and Chemical Reactivity

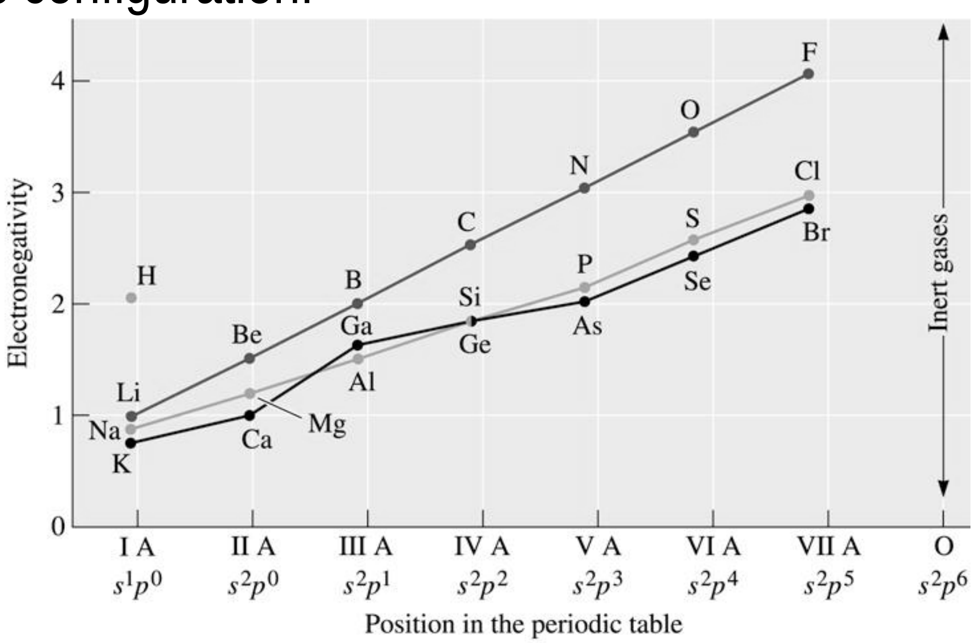
- Noble gases
- Less electronegative elements
- More electronegative elements



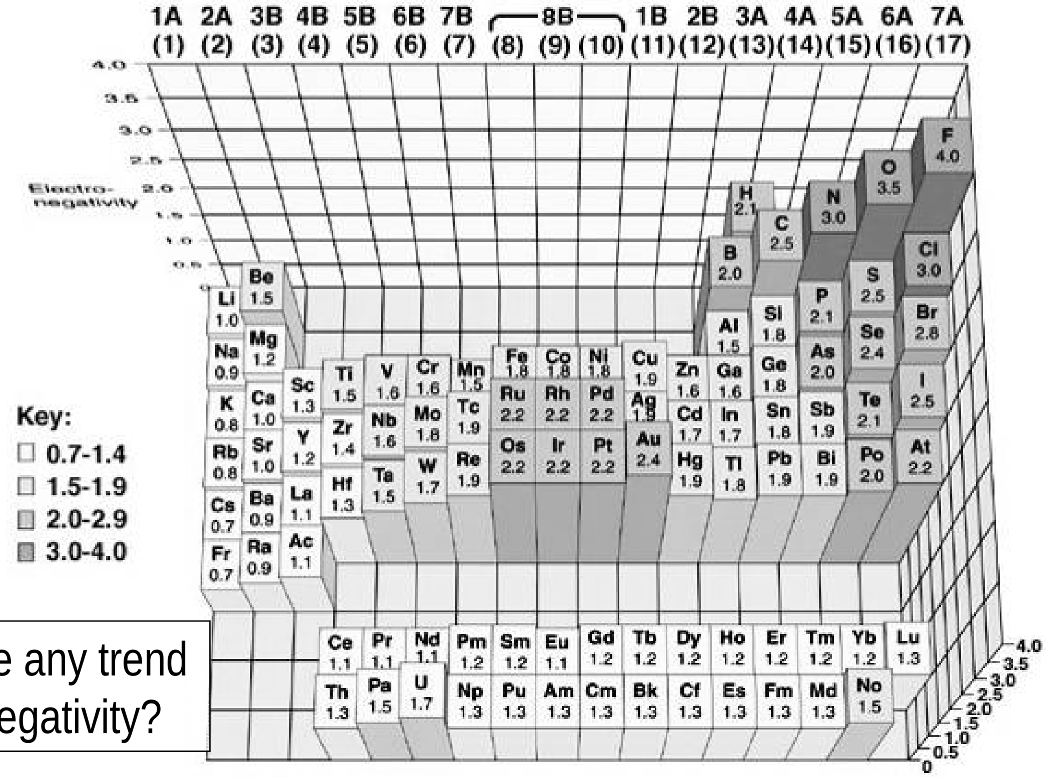
Then what is electronegativity?

- The tendency of an atom to attract an electron (or electron density)
- Most commonly used scale is Pauling's
- The most stable configuration of electrons is completely filled valence shells
- So, electronegativity controls how elements bond with each other

The electronegativities of selected elements relative to the position of the elements in the periodic table is related to the electronic configuration:



Pauling Electronegativities of the Elements

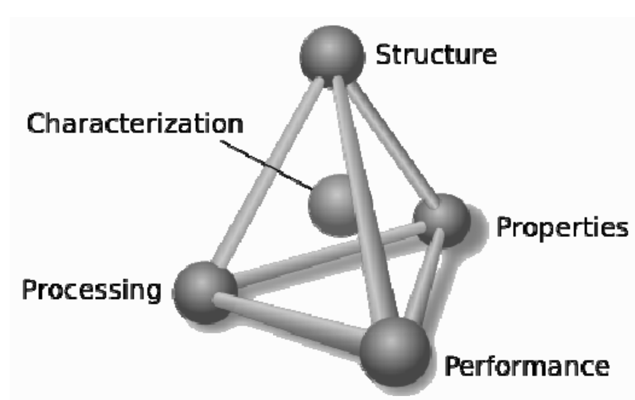


Do you see any trend in electronegativity?

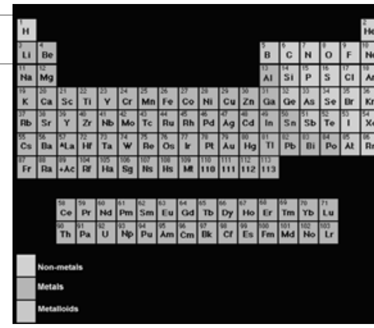
Atomic and Molecular Bonds

Remember: the nature of bonds defines the physical, chemical and mechanical properties of materials

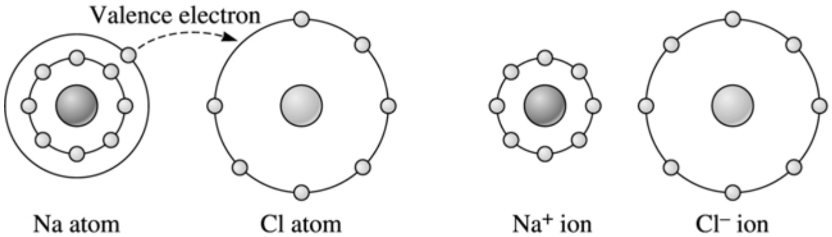
1. Ionic Bonds
2. Covalent Bonds
3. Metallic Bonds
4. Secondary Bonds:
   - -Permanent dipoles
   - -Fluctuating dipoles

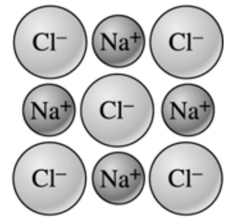


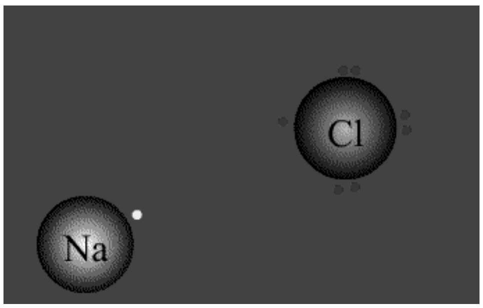
1. The ionization process



A $3s^1$ electron (Na) is transferred to a half-empty 3p orbital (Cl)







What happened to the ionic radii with respect to the atomic radii?

No bond is completely ionic, and some supposedly "ionic" compounds, especially of the transition metals, are particularly covalent in character

Common Ionic Bonds

- Metals combine with nonmetals & form ionic bonds by losing or gaining electrons to mimic closest Inert Gas (VIIIA).

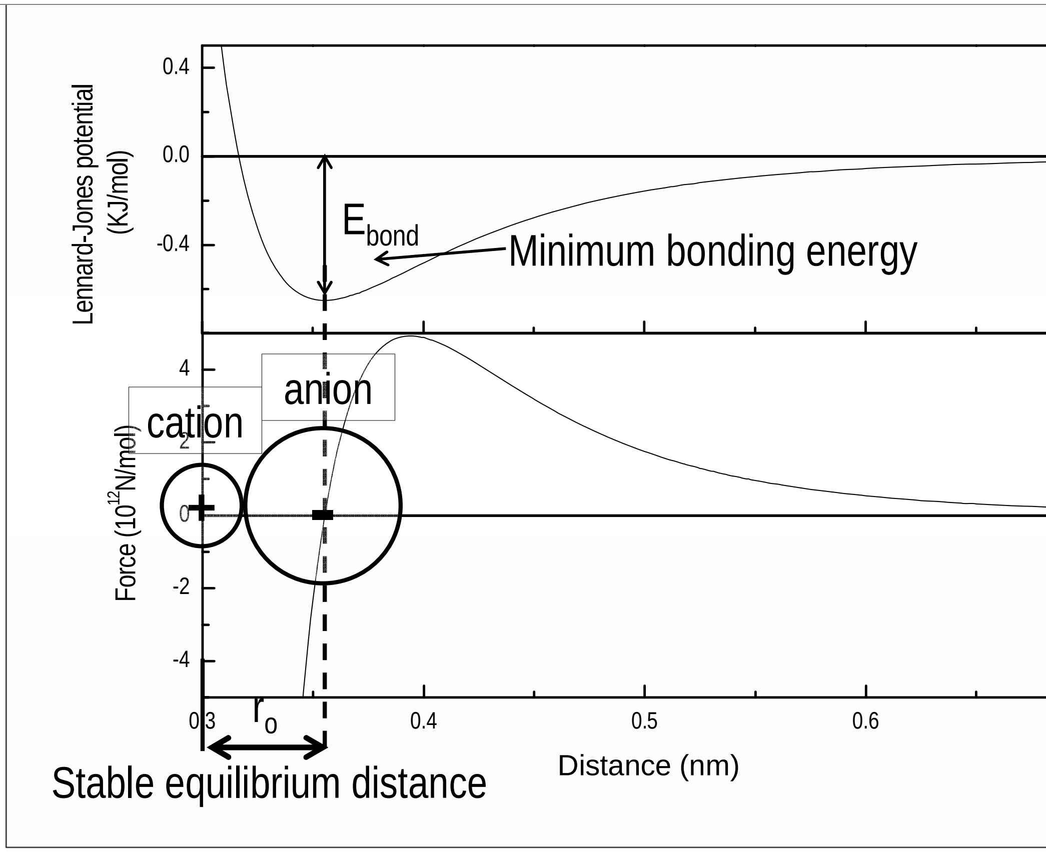
IA	- Na, K, Li, etc become +1 ions:	Na^+
IIA	- Ca, Mg, etc become +2 ions::	Ca^{+2}
IIIA	- Al, Ga become +3 ions:	Al^{+3}
VA	- N, P become -3 ions:	N^{-3}
VIA	- O, S become -2 ions:	O^{-2}
VIIA	- F, Cl, Br, I become -1 ions:	F^{-1}

Inert gas electronic configurations

Opposite ions attract in a ratio so that the product is neutral.

Homework: Give the formulas for the following element pairs and find applications of these compounds: Na & Br Ca & O Ba & I Al & O Br & I

All chemical bonds have energies & forces associated with them



$$E_A = -\frac{A}{r}$$

$$E_R = \frac{B}{r^n}$$

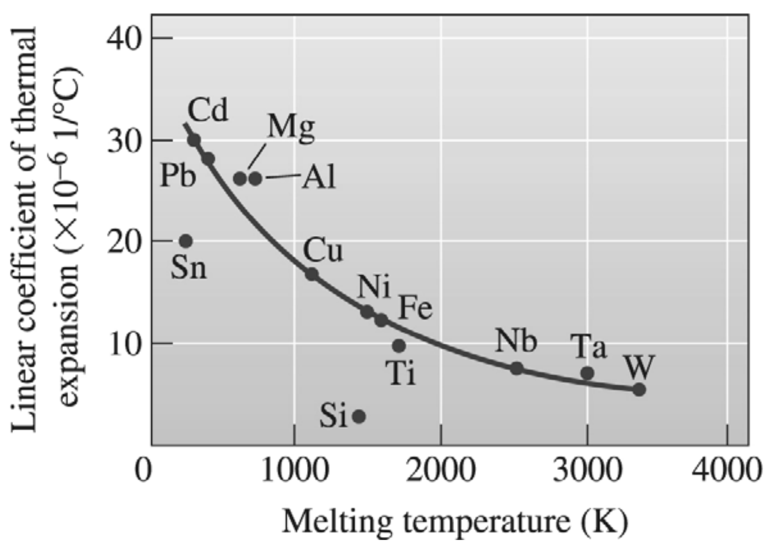
Interatomic energies and forces regulate important physical and mechanical properties of materials

- Melting points (energy curves)
- Thermal expansion coefficients (energy curves) *pages 791-793*

$$\alpha = \frac{\Delta \ell}{\ell_0 \cdot \Delta T}$$

In reality α varies with temperature ranges and allotropic changes

- Modulus of elasticity (force curves)

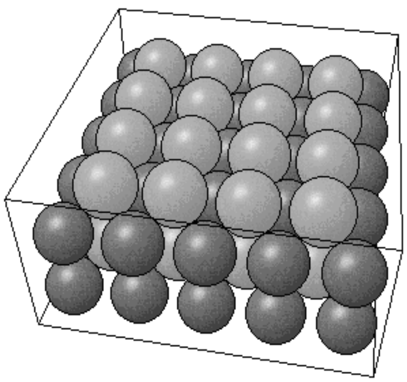


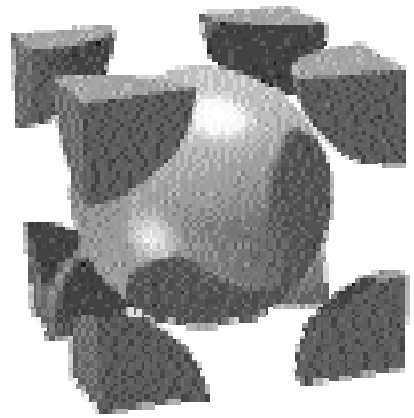
Dependence of α on MP of metals

Ion Arrangements in Ionic Solids

- Geometric Arrangements
- Electrical Neutrality

Cesium Chloride
CsCl Crystal

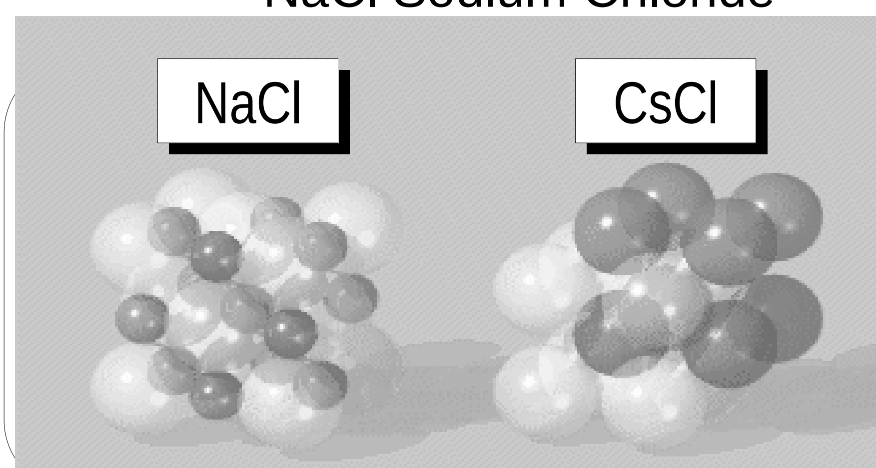




Let's introduce the concept of coordination number CN

Other Classical Example:

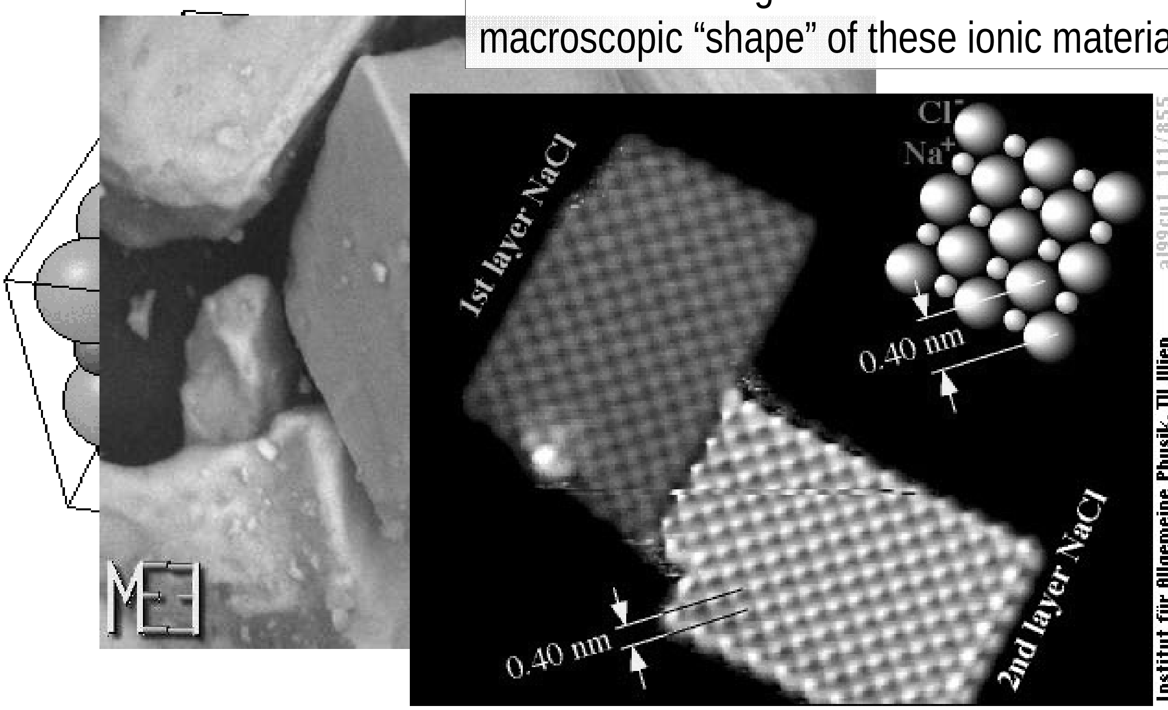
NaCl Sodium Chloride



Compare the NaCl crystal with the CsCl crystal

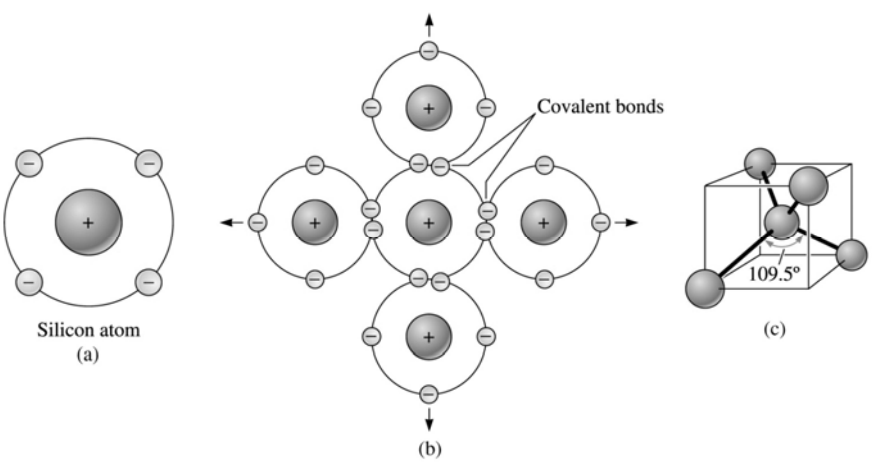
Yet more on NaCl

The atomic arrangement defines the macroscopic “shape” of these ionic materials

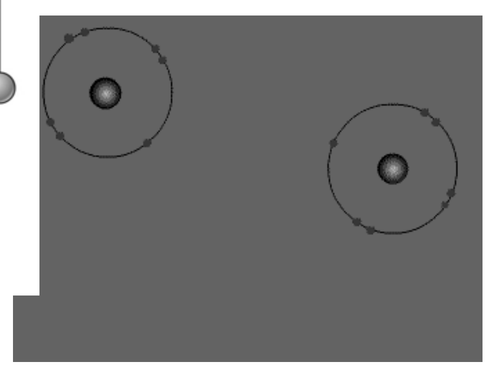


Periodic Table INGE 4001 - Engineering Materials

2. Covalent Bonds



The Silicon Example

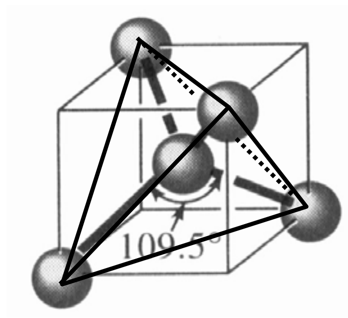


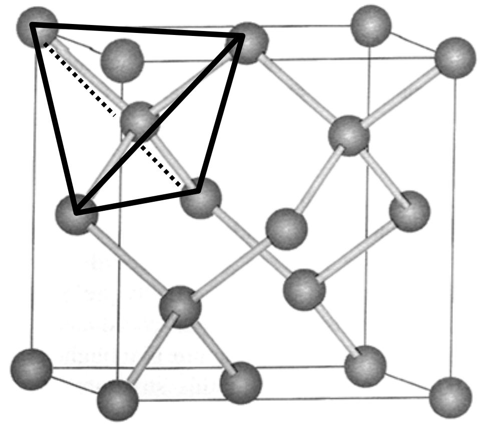
Atoms obtain inert gas configuration by sharing valence electrons

How about electronegativity?

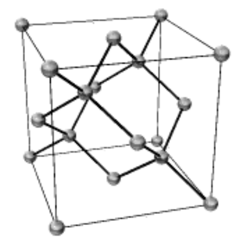
How would Ge and Si atoms bond?

The Silicon Example (cont.)



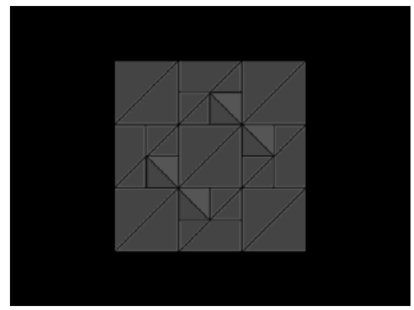


Notice the tetrahedra forming the cubic diamond unit cell



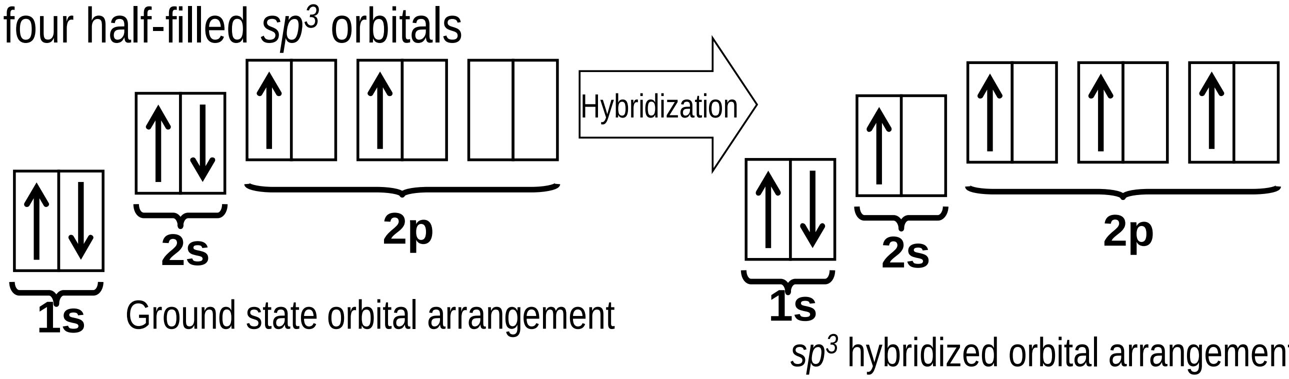
Covalent bonds are **directional**

Speculate about the formation of silica SiO_2



Covalent Bonds (cont.)

In the hybridization of carbon atoms, two half-filled *2p* orbitals become four half-filled sp^3 orbitals

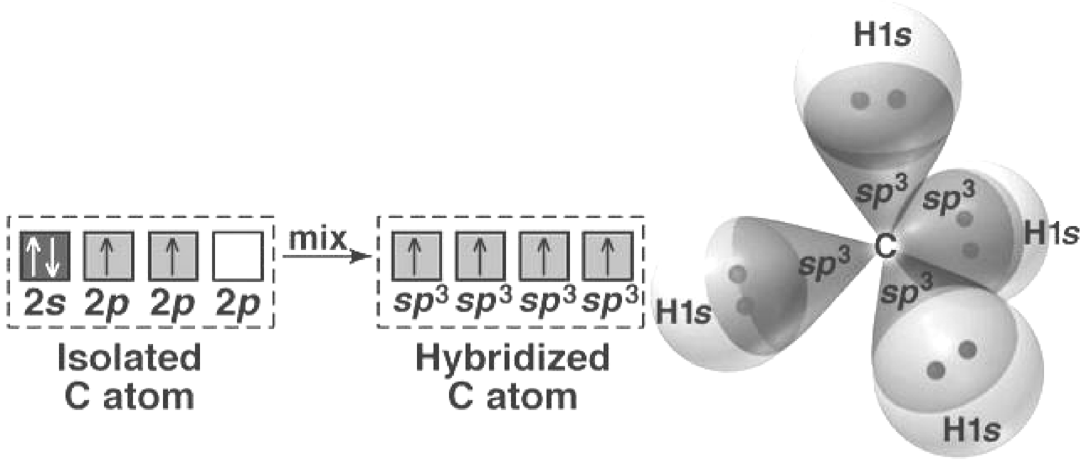


Sketch the hybridization of P to produce a molecule of PCl_5.

There are different types of hybridization in other systems: sp, sp^2, sp^3, sp^3d, sp^3d^2. What type is PCl_5? What about BF_3? SF_6? ClF_3? $BeCl_2$?

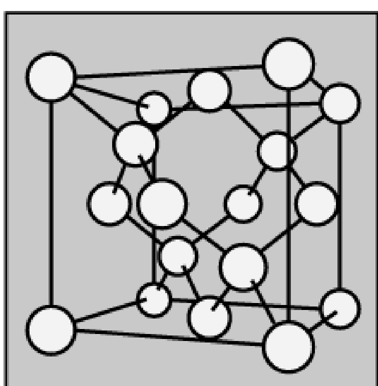
Please note that the system nomenclature indicates which orbitals are involved and how many electrons are in each orbital, e.g. sp^3d^2 means 1e$^-$ in *s*, 3e$^-$ in *p* and 2e$^-$ in *d*.

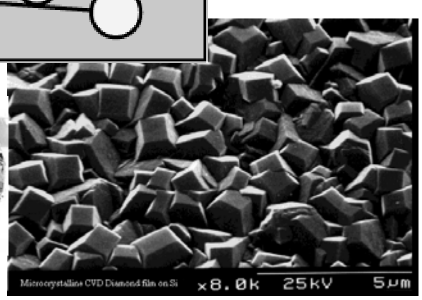
The sp^3 Hybrid Orbitals in CH_4



Then by replacing one H atom with OH → CH_3OH methanol

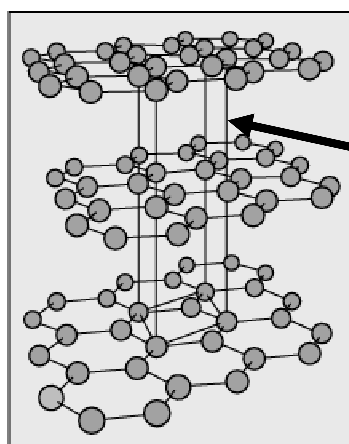
Different Carbon Arrangements





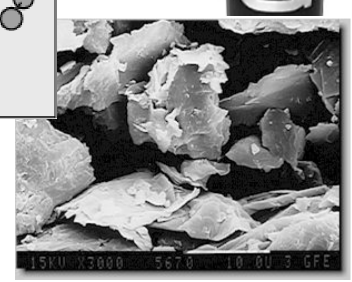
Diamond (cubic array)

Only σ (single bonds) among C atoms



The honecomb layers are called graphene.

Weaker secondary bonds



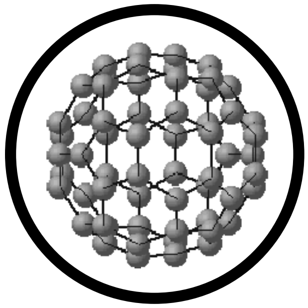
Graphite (hexagonal array)

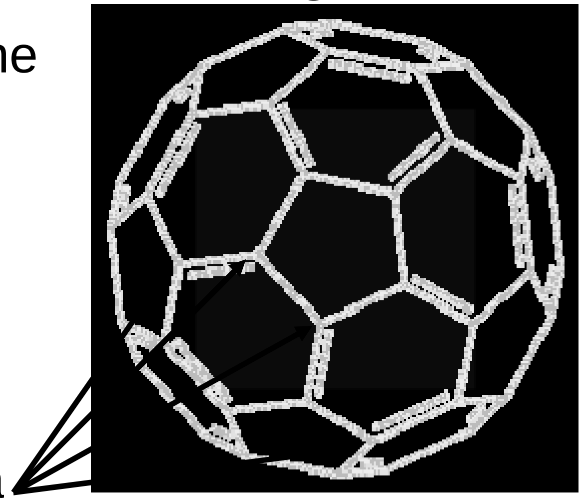
Alternate σ and π (double) bonds form the hexagons

And More Carbon Arrangements

Bucky Ball or Fullerene

C_{60}



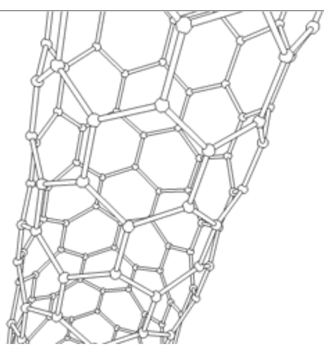


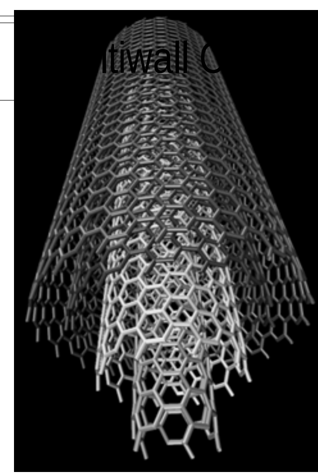
Each point is the location of a carbon atom

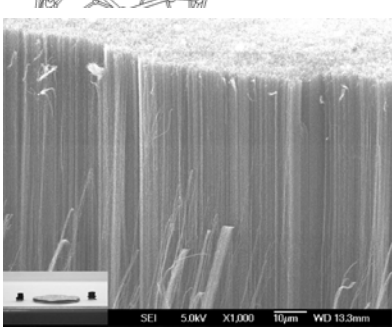
Note the positions of both σ and π bonds

What is the coordination number of each carbon atom?

Yet More Carbon Arrangements (Allotropy)







SWCNT grown on a silicon substrate: low reflexivity material