Types of Bonding

Primary bonding: e- are transferred or shared Strong (100-1000 KJ/mol or 1-10 eV/atom).

 Ionic: Strong Coulomb interaction among negative atoms (have an extra electron each) and positive atoms (lost an electron). Example - $Na^{+}Cl^{-}$

 Covalent: electrons are shared between the molecules, to saturate the valency. Example - H2

 Metallic: the atoms are ionized, losing some electrons from the valence band. Those electrons form an electron sea, which binds the charged nuclei in place.

Secondary Bonding: no e- transferred or shared Interaction of atomic/molecular dipoles Weak (< 100 KJ/mol or < 1 eV/atom)

 Fluctuating Induced Dipole (inert gases, H_2, Cl_2…)

 Permanent dipole bonds (polar molecules - H_2O, HCl...)

 Polar molecule-induced dipole bonds (a polar molecule induces a dipole in a nearby nonpolar atom/molecule)

Ionic Bonding

Ionic Bonding is typical for elements that are situated at the horizontal extremities of the periodic table.

Atoms from the left (metals) are ready to give up their valence electrons to the (non-metallic) atoms from the right that are happy to get one or a few electrons to acquire stable or noble gas electron configuration.

As a result of this transfer mutual ionization occurs: *atom that gives up electron(s) becomes positively charged ion (cation), atom that accepts electron(s) becomes negatively charged ion (anion).*

Formation of ionic bond:

1. Mutual ionization occurs by electron transfer

• Ion = charged atom

• Anion = negatively charged atom

• Cation = positively charged atom

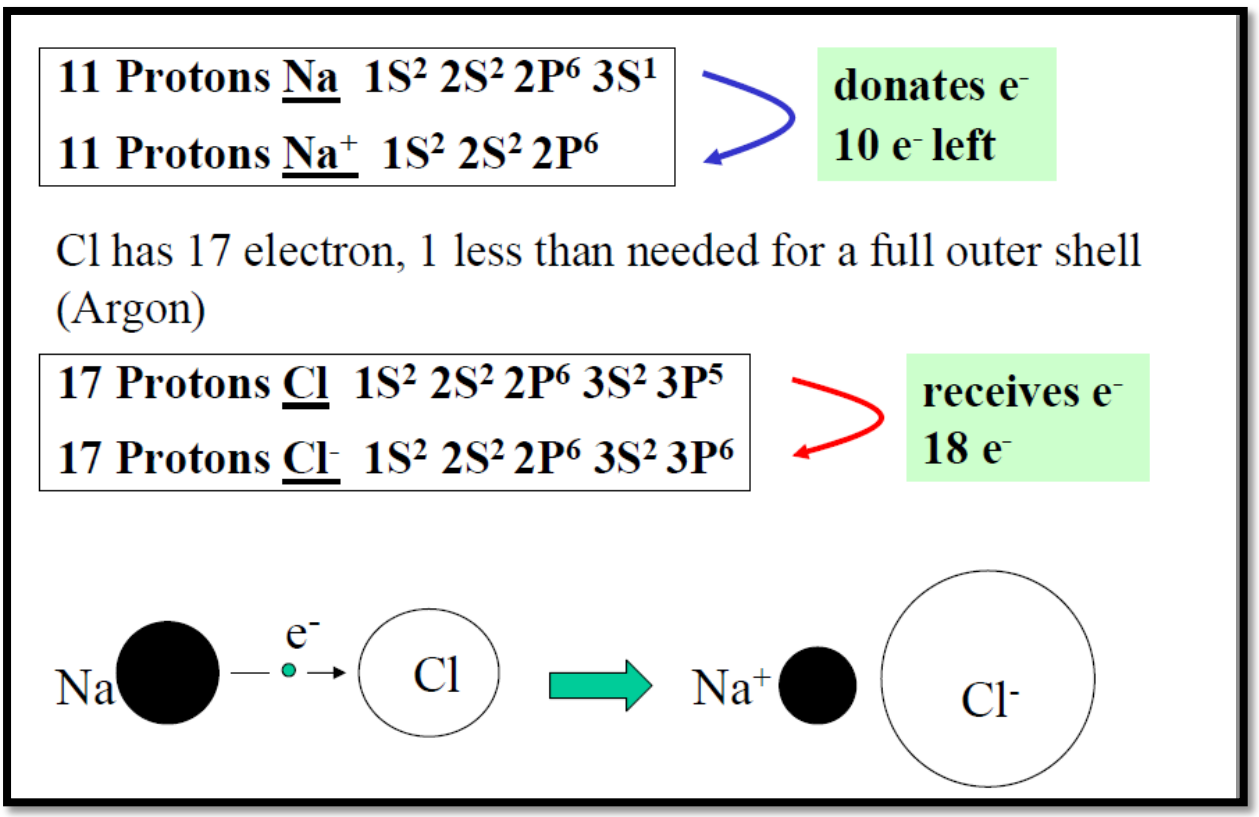
2. Ions are attracted by strong coulombic interaction

• Oppositely charged atoms attract each other

• An ionic bond is non-directional (ions may be attracted to one another in any direction).

***Example*:** table salt (NaCl)

Na has 11 electrons, 1 more than needed for a full outer shell .



• Electron transfer reduces the energy of the system of atoms, that is, electron transfer is energetically favorable

• Note relative sizes of ions: Na shrinks and Cl expands

Any mechanical force that tries to disturb the electrical balance in an ionic crystal meets strong resistance: ionic materials are strong and brittle. In some special cases,

however, significant plastic deformation can be observed, e.g. NaCl single crystals can be bent by hand in water.

Covalent Bonding

In covalent bonding, electrons are shared between the molecules, to saturate the valency.

In this case the electrons are not transferred as in the ionic bonding, but they are localized between the neighboring ions and form directional bond between them.

The ions repel each other, but are attracted to the electrons that spend most of the time in between the ions.

Formation of covalent bonds:

• Cooperative sharing of valence electrons

• Can be described by orbital overlap

• Covalent bonds are HIGHLY directional

• Bonds - in the direction of the greatest orbital overlap

• Covalent bond model: an atom can covalently bond with

at most 8-N', N' = number of valence electrons

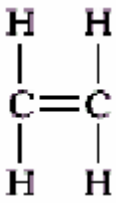
Example: Cl_2 molecule. Z_{Cl} =17 (1S2 2S2 2P6 3S2 3P5)

N' = 7, 8 - N' = 1 → can form only one covalent bond

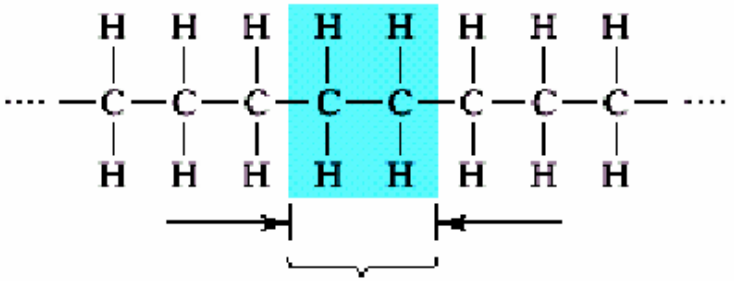
Example: Carbon materials. Zc = 6 (1S2 2S2 2P2)

N' = 4, 8 - N' = 4 → can form up to four covalent bonds

ethylene molecule:



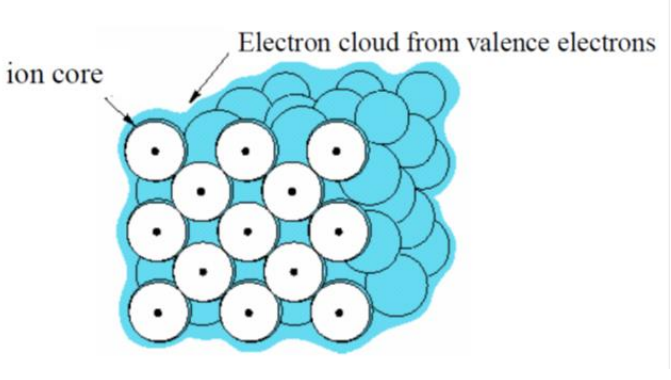
polyethylene molecule:



Metallic Bonding

Valence electrons are detached from atoms, and spread in an 'electron sea' that "glues" the positive ions together.

• A metallic bond is non-directional (bonds form in any direction) → atoms



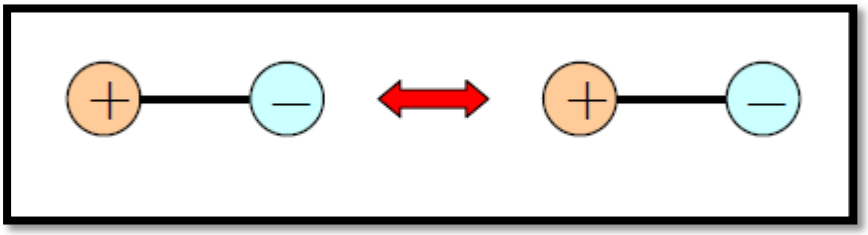
The "bonds" do not "break" when atoms are rearranged – metals can experience a significant degree of plastic deformation.

Examples of typical metallic bonding: Cu, Al, Au, Ag, etc.

Transition metals (Fe, Ni, etc.) form mixed bonds that are comprising of metallic bonds and covalent bonds involving their 3d-electrons. As a result the transition metals are more brittle (less ductile) that Au or Cu.

Secondary Bonding

Secondary = van der Waals = physical (as opposite to chemical bonding that involves e- transfer) bonding results from interaction of atomic or molecular dipoles and is weak, ***~0.1 eV/atom or ~10 kJ/mol.***



- Permanent dipole moments exist in some molecules (called **polar molecules**) due to the asymmetrical arrangement of positively and negatively regions (HCl, H2O).
- Bonds between adjacent polar molecules – **permanent dipole bonds** – are the strongest among secondary bonds.
- Polar molecules can induce dipoles in adjacent non-polar molecules and bond is formed due to the attraction between the permanent and induced dipoles.
- Even in electrically symmetric molecules/atoms an electric dipole can be created by fluctuations of electron density distribution.
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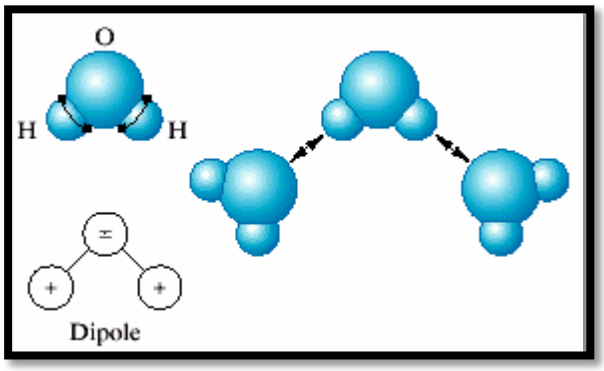
- Fluctuating electric field in one atom A is felt by the electrons of an adjacent atom, and induce a dipole momentum in this atom.
- This bond due to fluctuating induced dipoles is the weakest (inert gases, H2, Cl2).

Example: hydrogen bond in water:

The H end of the molecule is positively charged and can bond to the negative side of another H_2O molecule (the O side of the H_2O dipole)



“Hydrogen bond” – secondary bond formed between two permanent dipoles in adjacent water molecules.

Molecules: Primary bonds inside, secondary bonds among each other.

Bonding in real materials

In many materials more than one type of bonding is involved (ionic and covalent in ceramics, covalent and secondary in polymers, covalent and ionic in semiconductors.

Examples of bonding in Materials:

- Metals: Metallic
- Ceramics: Ionic / Covalent
- Polymers: Covalent and Secondary
- Semiconductors: Covalent or Covalent / Ionic