Lecture: P1_Wk1_L1

IntraMolecular Interactions

Distinguish between
IntraMolecular (within a molecule)
and
InterMolecular (between molecules)

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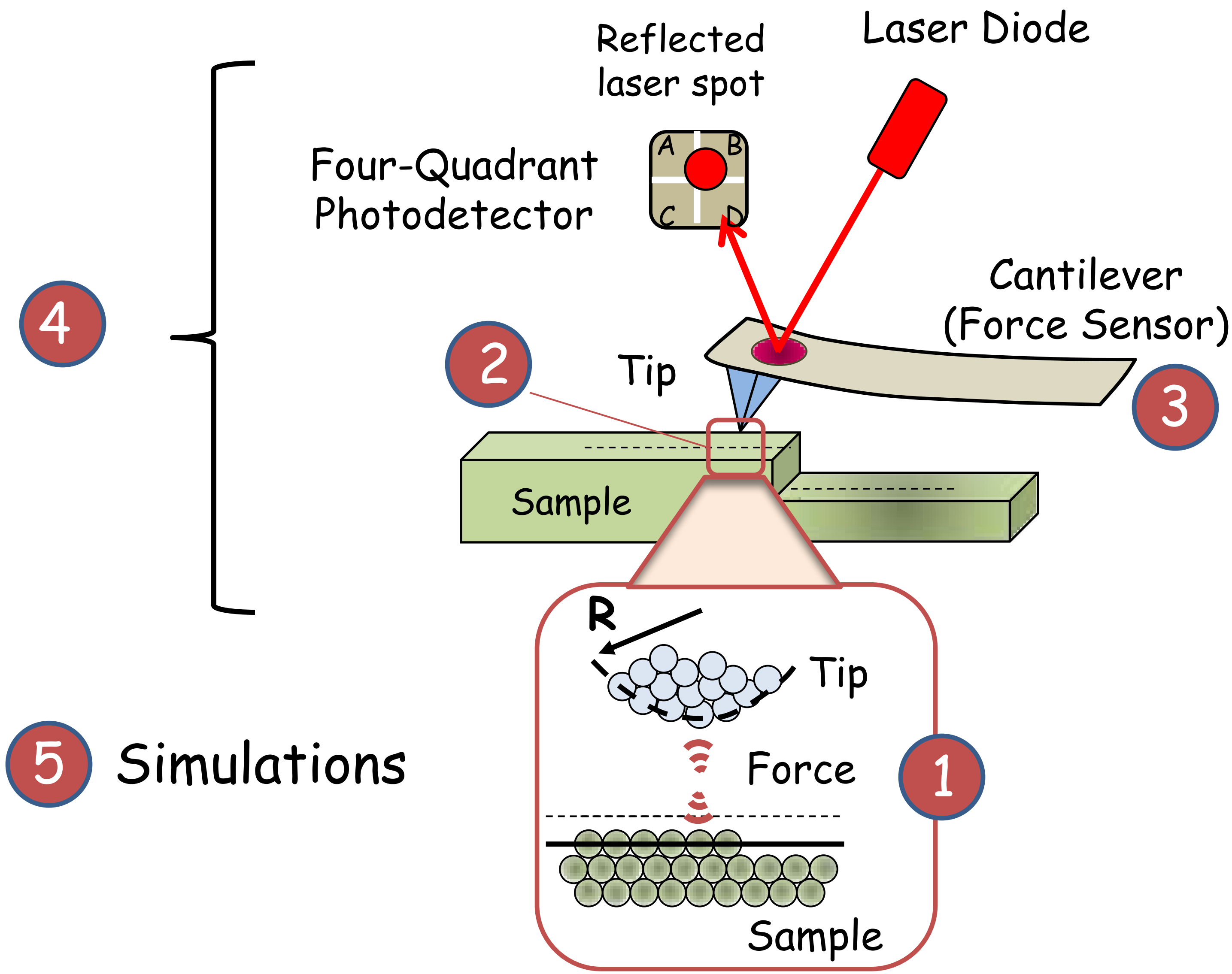
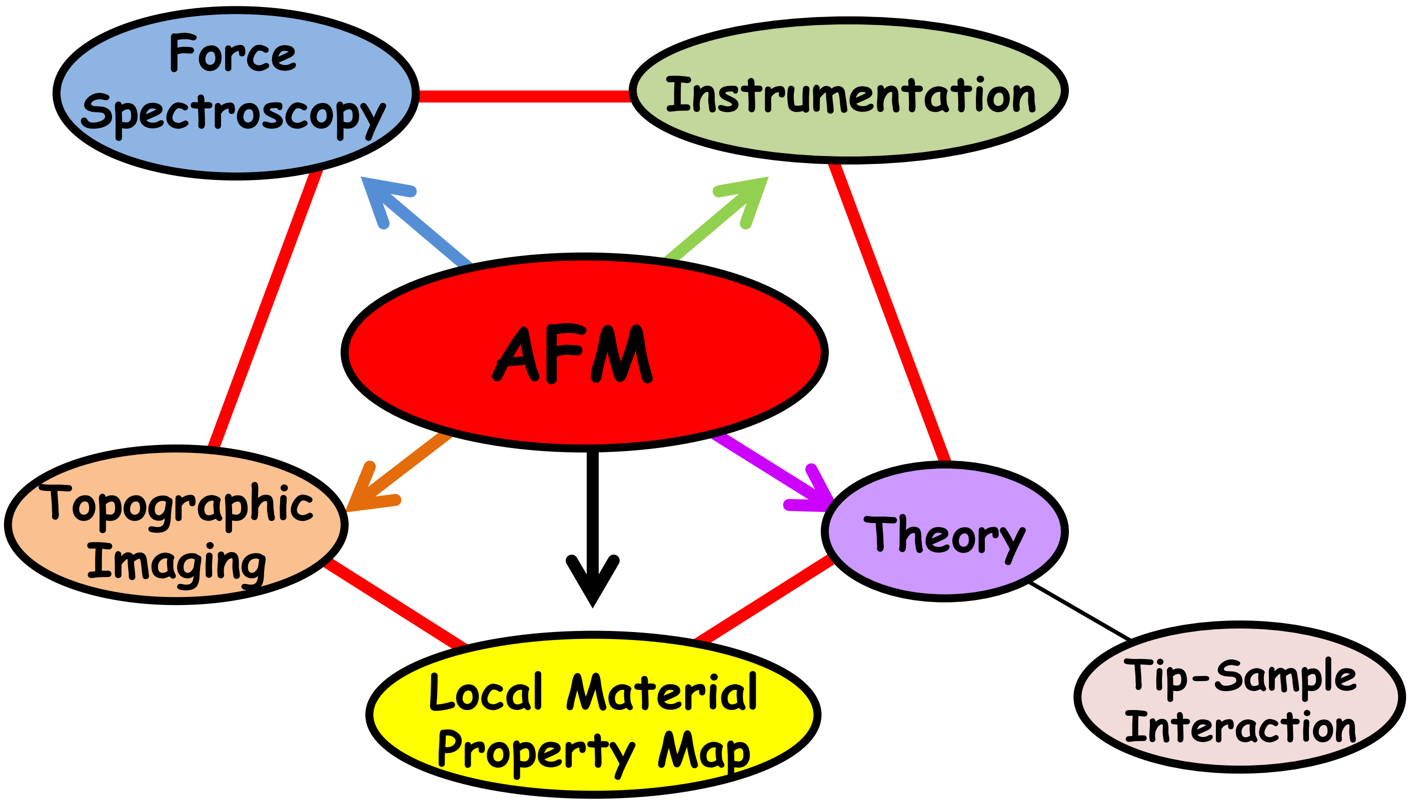
This course is about the Atomic Force Microscope



Week 1



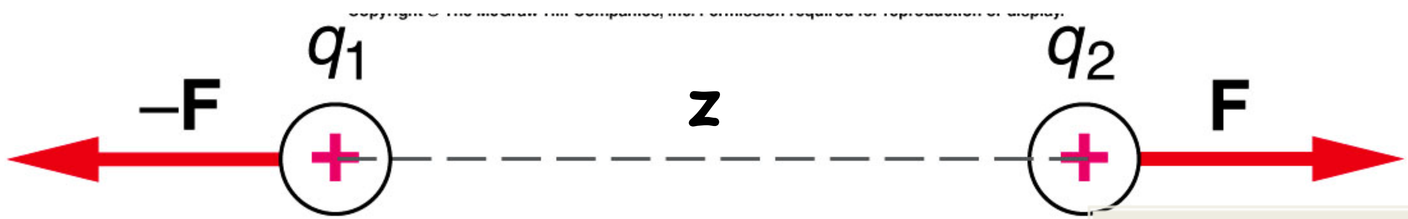
Force Spectroscopy
Instrumentation
AFM
Topographic Imaging
Theory
Local Material Property Map
Tip-Sample Interaction

The Origin of Intramolecular Interactions is Electrostatic:

Coulomb's Law – Classical Picture

Point charges ONLY!

The charges are stuck down!



In vacuum

$$|\vec{F}| = \frac{1}{4\pi\varepsilon_o}\frac{q_1 q_2}{z^2} = k\frac{q_1 q_2}{z^2}$$

$$\varepsilon_o = 8.85 \times 10^{-12}\ C^2 / Nm^2$$

$$k = 9 \times 10^9\ Nm^2 / C^2$$

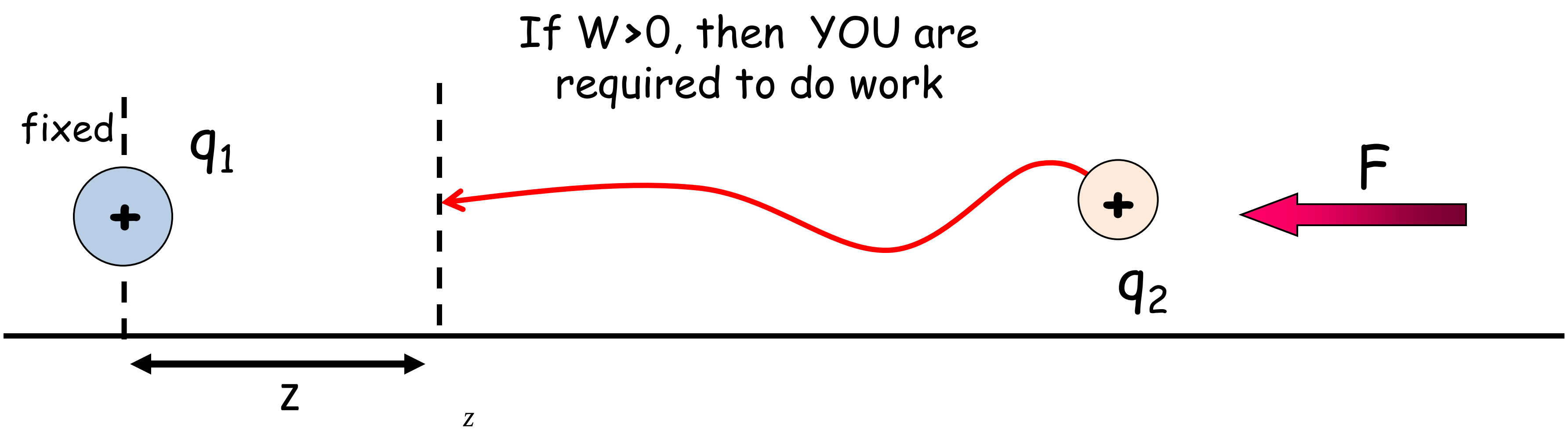
Force is a vector

With dielectric in between,

$\varepsilon_o \longrightarrow \kappa\varepsilon_o$

κ (dielectric constant)>1

Energy Is Required to Assemble Charges



$$W \equiv \int_{\infty}^{z} \vec{F} \bullet d\vec{\ell}$$

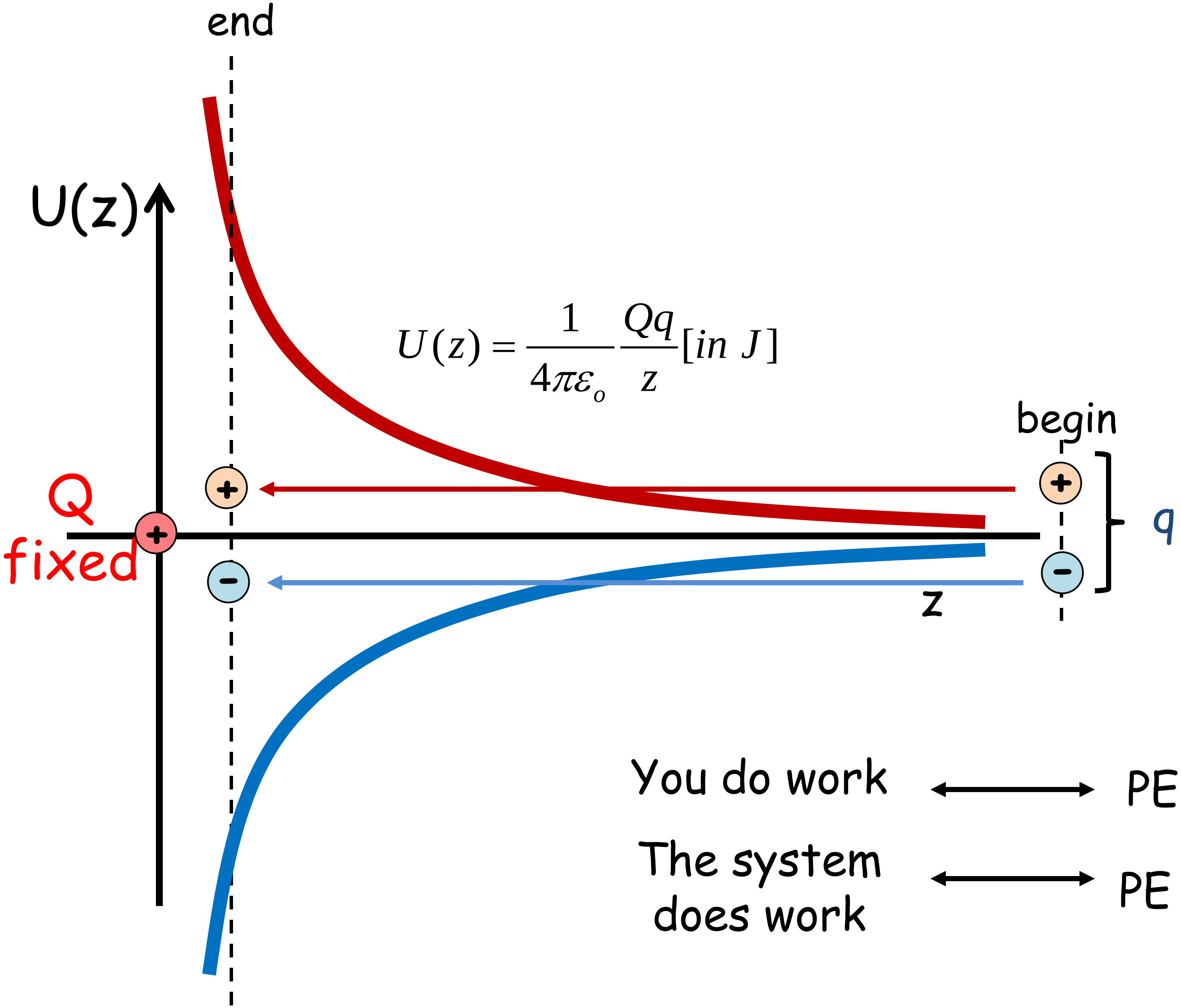
$$Electrostatic\ Potential\ Energy = U(z) \equiv -W$$

For two point charges a distance z apart:

$$U(z) = \frac{1}{4\pi\varepsilon_o}\frac{q_1 q_2}{z}[in\ J]$$

$$useful\ because \quad F(z) = -\frac{\partial U}{\partial z} \quad (recover\ Coulomb's\ Law)$$

Electrostatic Potential Energy is a signed quantity



$$U(z) = \frac{1}{4\pi\varepsilon_o}\frac{Qq}{z}[in\ J]$$

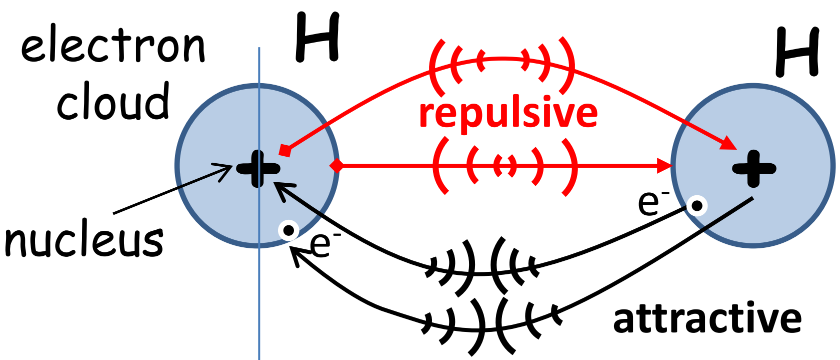
Push "+q" charge with external force

You do work ⟷ PE increases

The system does work ⟷ PE decreases

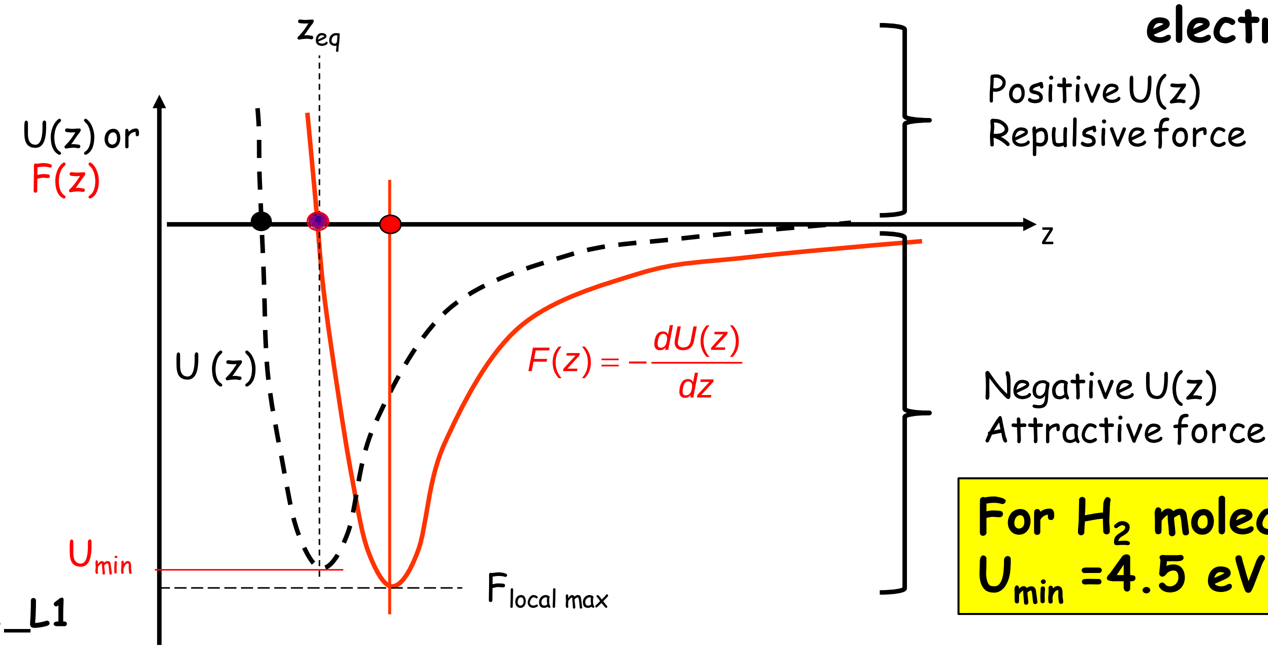
IntraMolecular (within a molecule) Electrostatic Potential

electrostatic forces lead to the formation of stable molecules



Summing the four contributions:

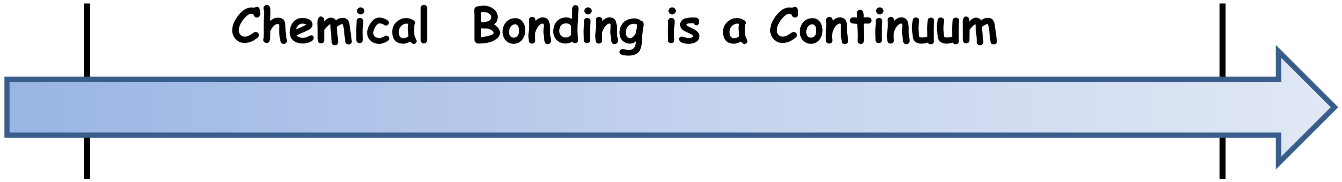
The chemical "bond" that forms between two H atoms is due to an overall net electrical attraction.



For H_2 molecule near 300K: U_{min} =4.5 eV and z_{eq} =75 pm

IntraMolecular Forces Lead to Chemical Bonding (where are the electrons?)

Chemical Bonding is a Continuum

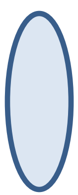


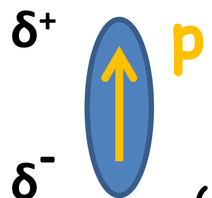
Totally Covalent:
equal electron sharing between **identical** atoms

(di)Polar Covalent:
unequal electron sharing between **dissimilar** atoms

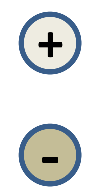
Ionic:
complete electron transfer between dissimilar atoms

No permanent electric dipole (non-polar molecule)





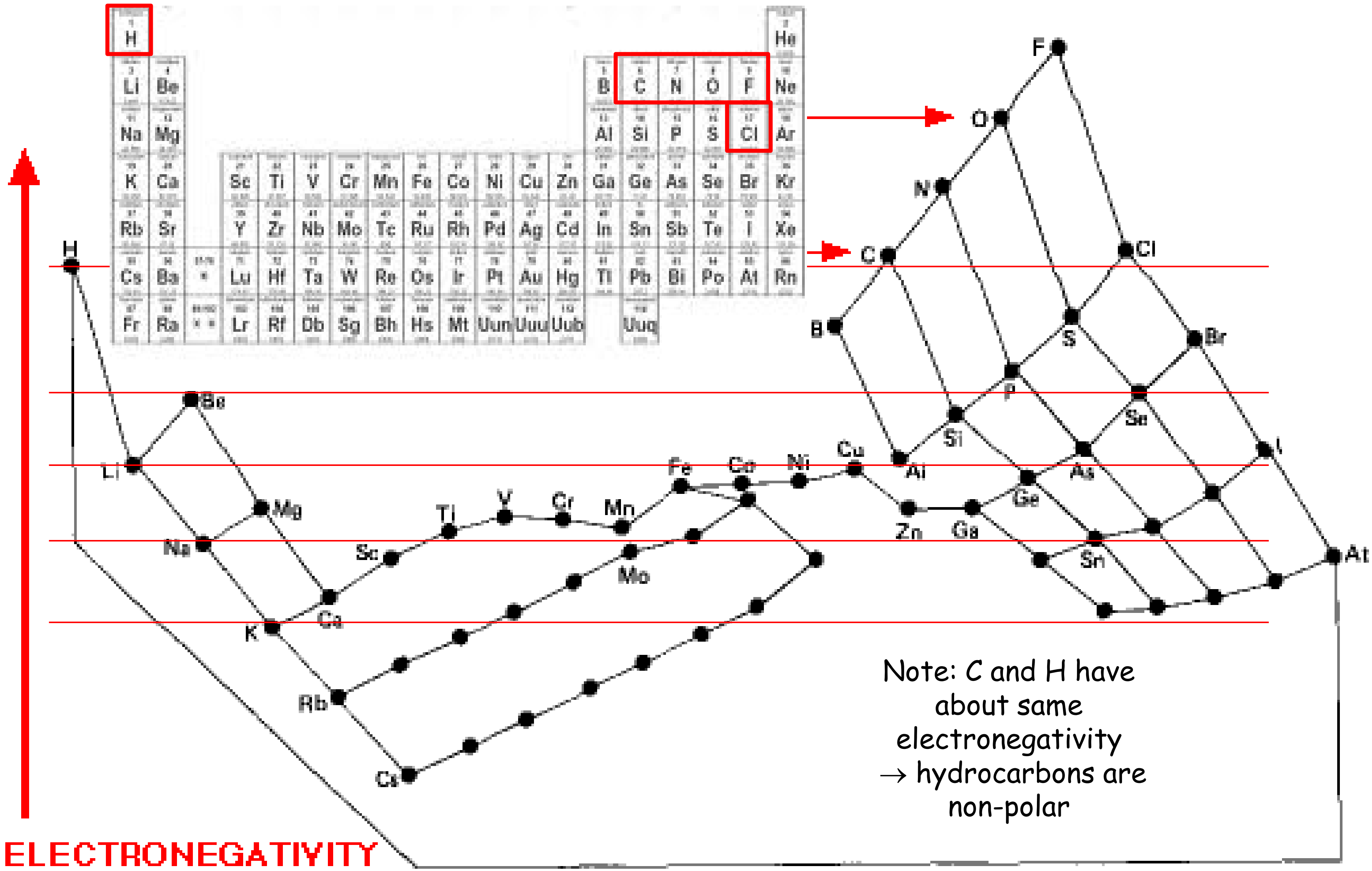
Permanent electric dipole moment, p (dipolar molecule)



Net charge transfer (ion)

Note: " δ^+ " means "slightly positive"

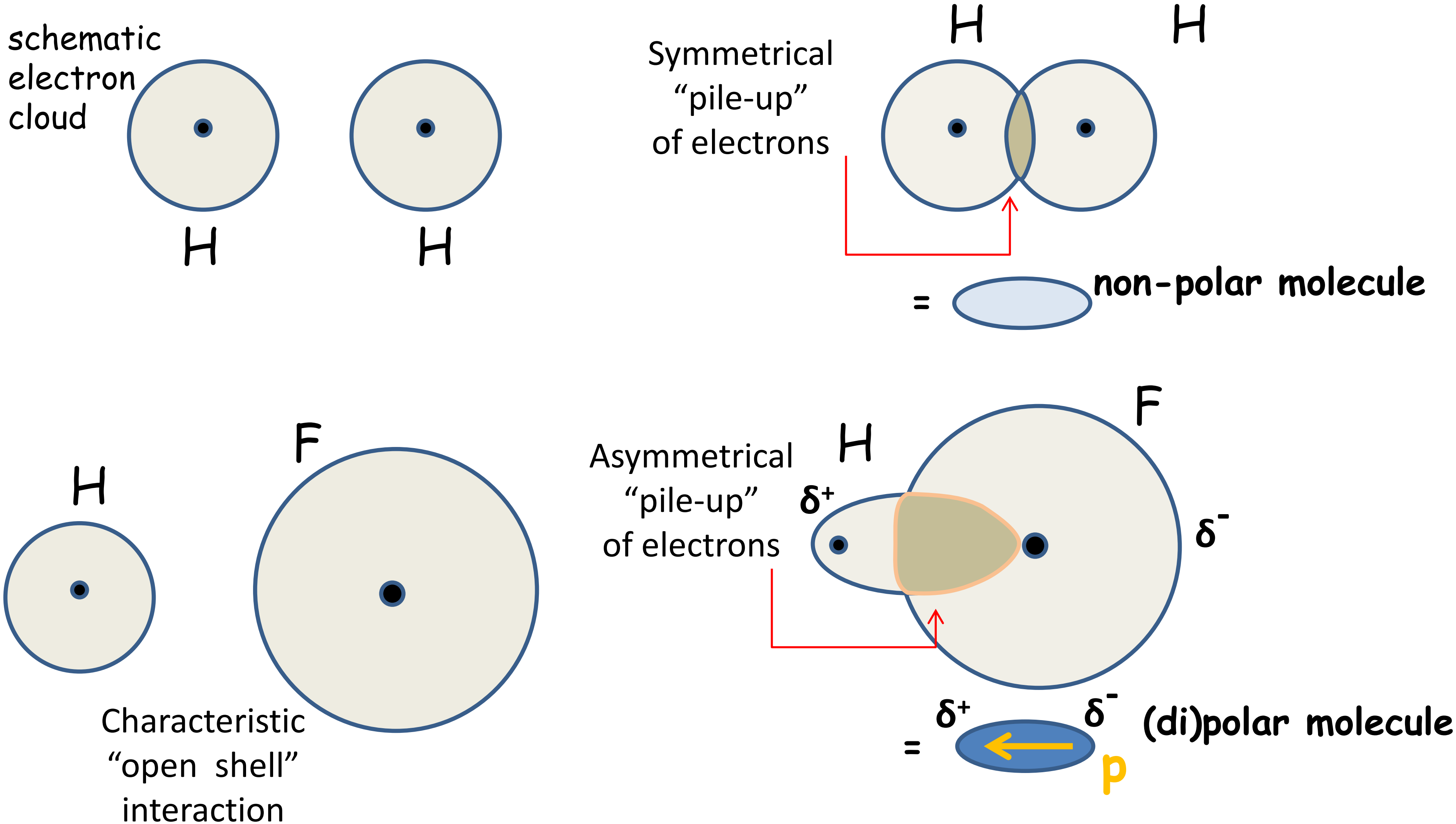
Electronegativity – measures the ability of an atom in a molecule to attract electrons



Note: C and H have about same electronegativity → hydrocarbons are non-polar

http://users.rcn.com/jkimball.ma.ultranet/BiologyPages/

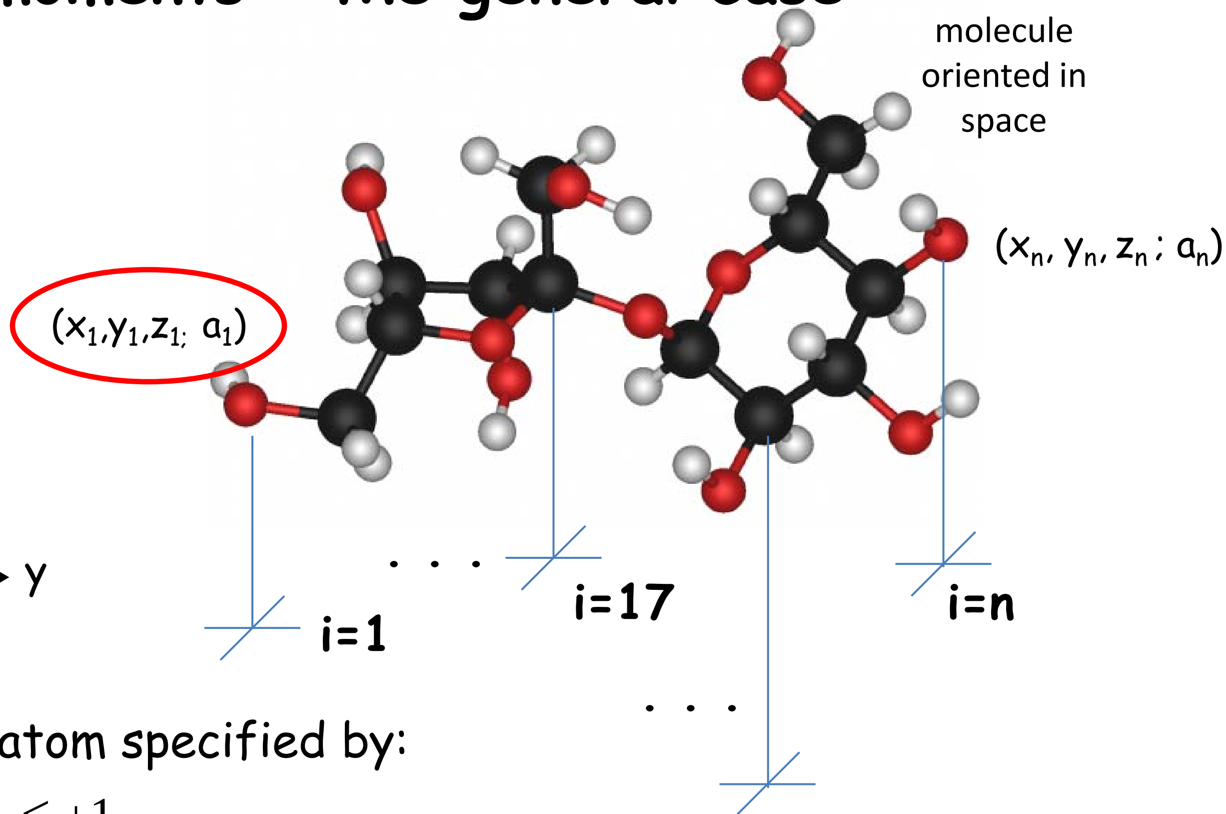
Simple examples of non-(di)polar covalent and (di)polar covalent molecules

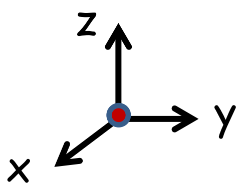


P1_Wk1_L1

Molecular dipole moments – the general case

Need to know:





partial charge on each atom specified by:

$$\delta q_i = a_i \left| e^- \right| \qquad -1 \le a_i \le +1$$

$$p_x = \sum_i x_i\, \delta q_i \quad p_y = \sum_i y_i\, \delta q_i \quad p_z = \sum_i z_i\, \delta q_i \quad \left|\vec{p}\right| = \sqrt{p_x^2 + p_y^2 + p_z^2}$$

Values for (x_i, y_i, zi; a_i) are obtained from quantum chemistry calculation.

If $\Sigma a_i=0$ (electrically neutral molecule), then calculation of (p_x, p_y, p_z) is independent of co-ordinate origin.

Stick-ball model: http://scienceray.com/biology/carbohydrates-2/

InterMolecular Interactions

Because electrically neutral molecules can have a dipole moment, interactions between molecules **(InterMolecular Forces)** are non-zero. These InterMolecular Forces cause molecules to condense and form a liquid or a solid.

The **strength of intermolecular forces** determines such things as the boiling point, surface tension, and viscosity of liquids.

Classifying InterMolecular Interactions

Ultimately, all intermolecular forces act between charged species:

- If molecule has net electrical charge - **long range Coulomb interaction**

- If molecule has polarized electrical charge – **dipole-dipole interaction**.

- Electric field from one molecule may induce small changes in electron distribution of nearby molecule – **induction**.

- Instantaneous dipole associated with rapid electron movement in one molecule becomes correlated with rapid electron movement in another molecule – **dispersion**.