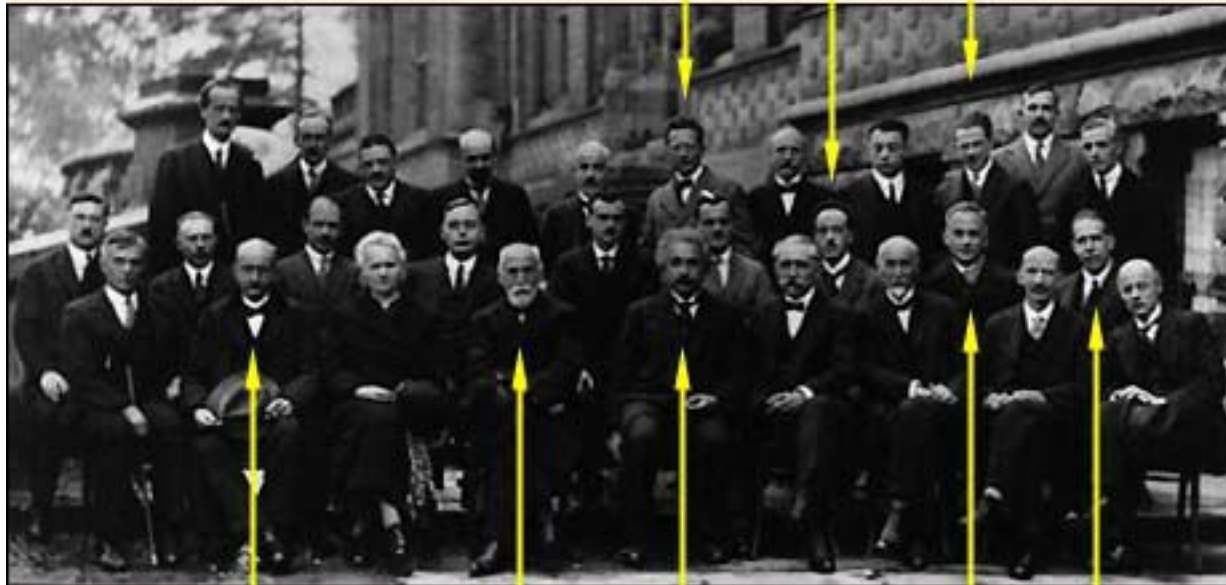


Structure of an atom: Agreed upon by experimentalists and theoreticians.

Today's knowledge of an atom comes from meetings like

The Solvay Congress of 1927



Werner Heisenberg

Louis de Broglie

Erwin Schrödinger

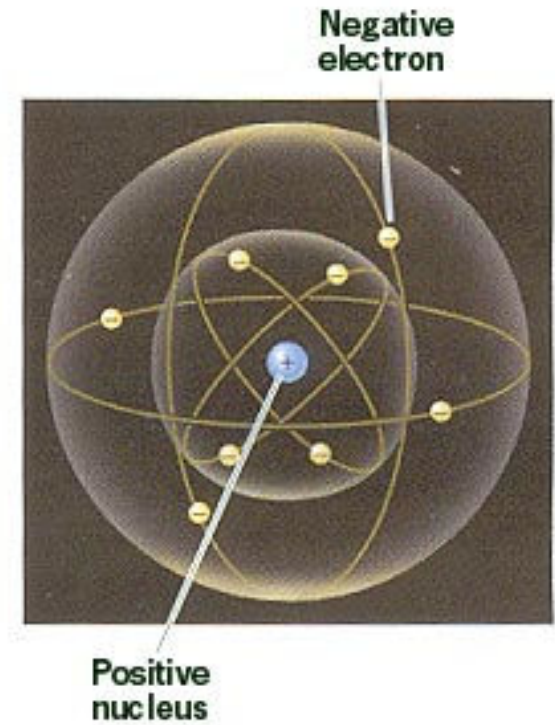
H. A. Lorentz

Max Born

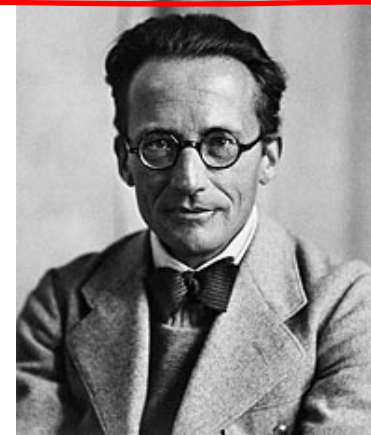
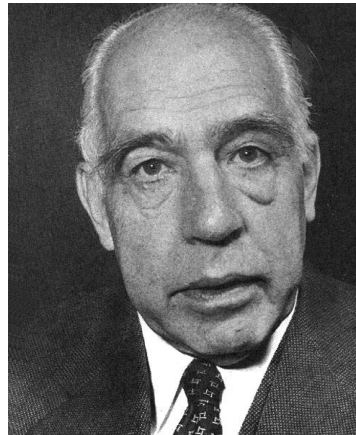
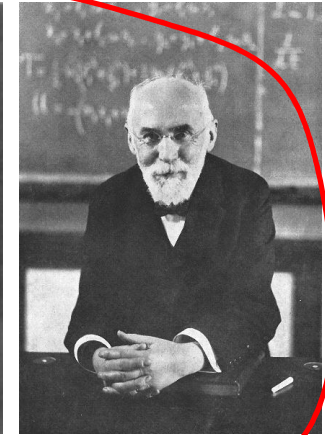
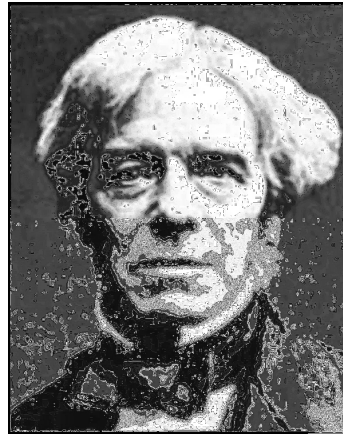
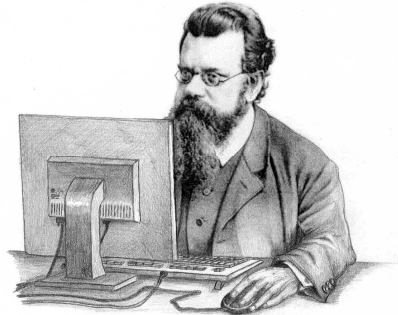
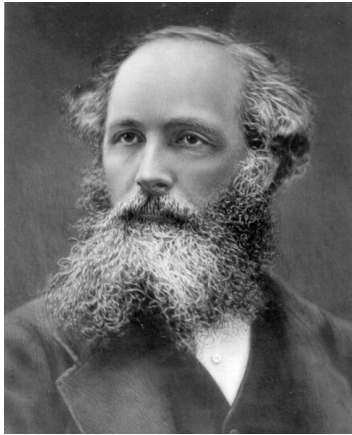
Max Planck

Einstein

Niels Bohr



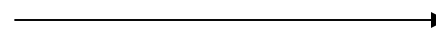
Mid 1800s



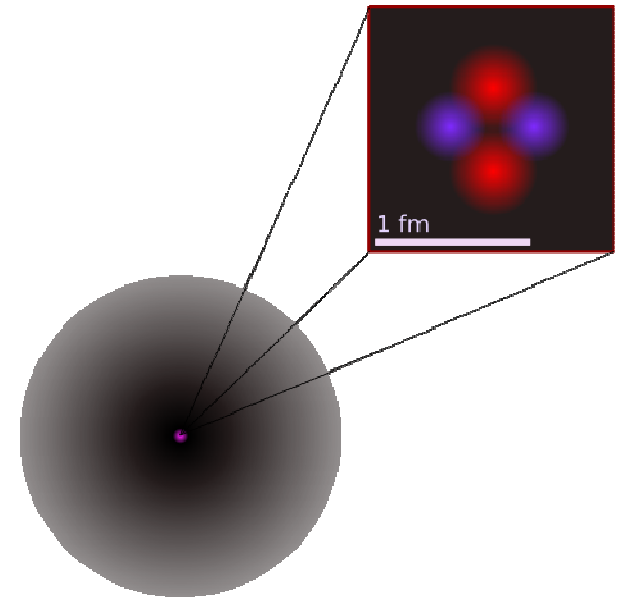
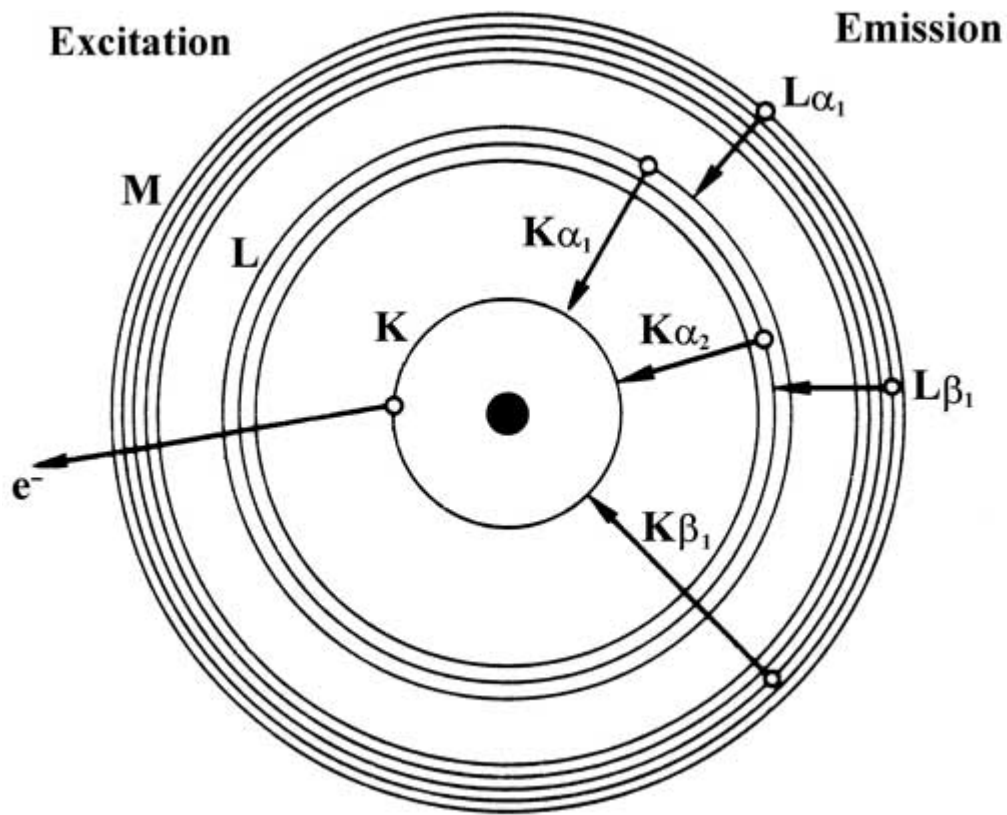
1930s

From $F = m \times a$ to
Newtonian
Mechanics

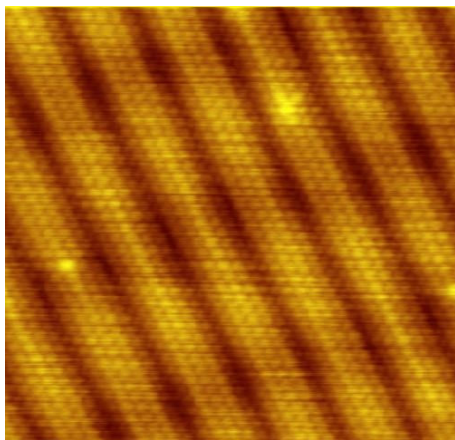
$E = \hbar \times \omega$
Quantum
Mechanics



Prediction of new
materials using
computers
(Late 1990s)

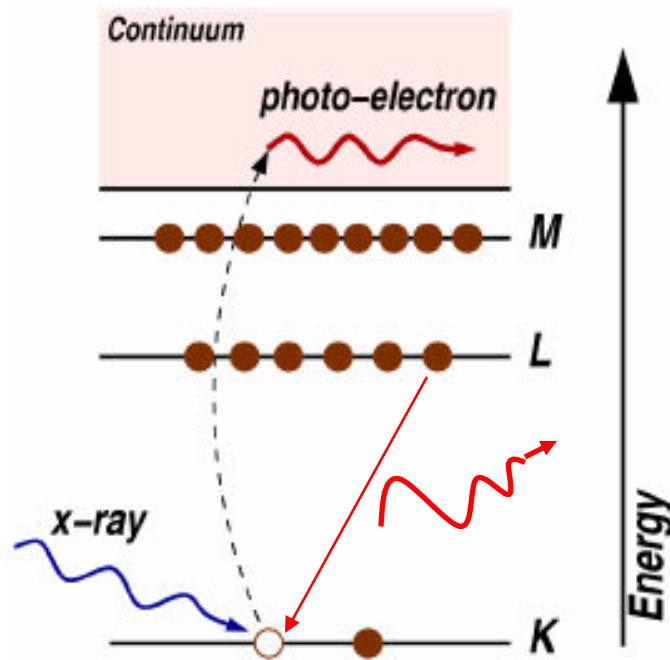


1 Ångström (=100,000 fm)



STM surface image of gold

Using atoms as a footprint of chemistry:



Fact: electrons exist in discrete orbits around the nuclei. ↓

Atomic nuclei are well-distinguishable due to their proton content. ↓

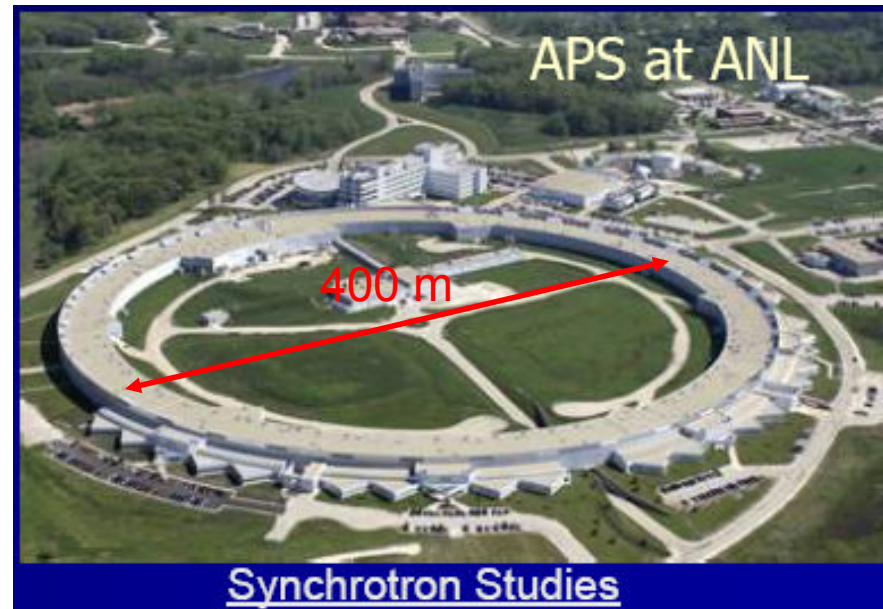
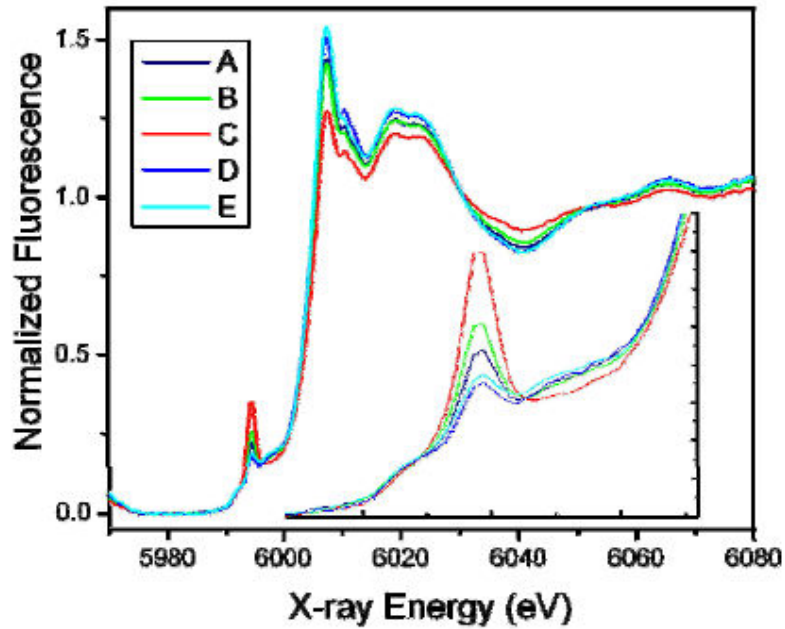
Then electron orbits of different atoms must be at different energies.

$$h\lambda = \Phi + \text{Kin. En.} \quad (\text{Eqn. of Einstein})$$

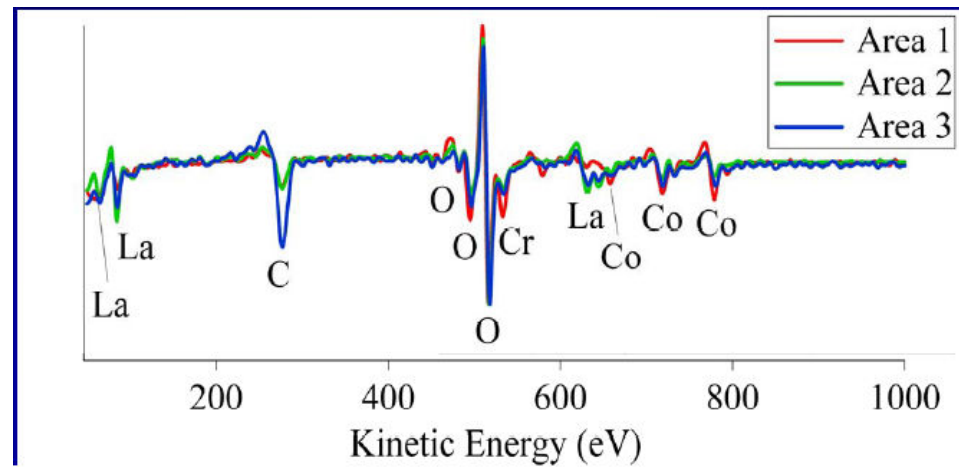
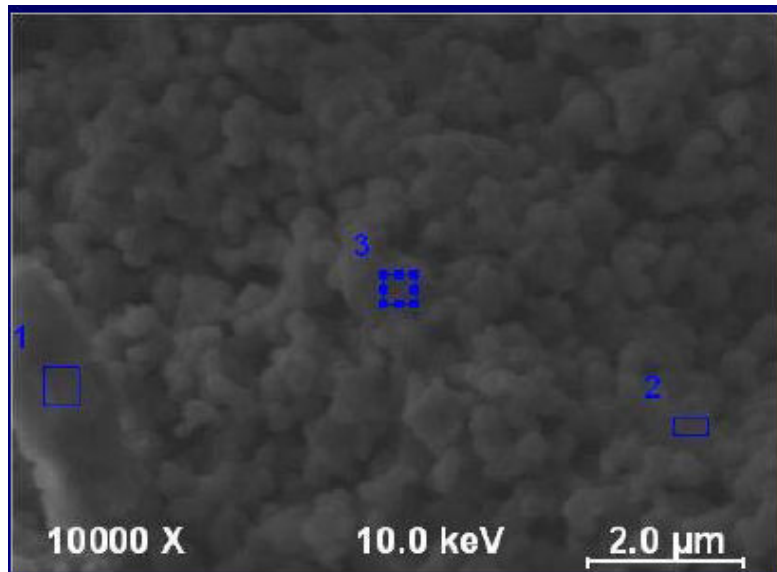
Figure 2.1: The photoelectric effect, in which an x-ray is absorbed and a core-level electron is promoted out of the atom.

Energy of incoming radiation = Energy of photo electron + Energy difference K-L

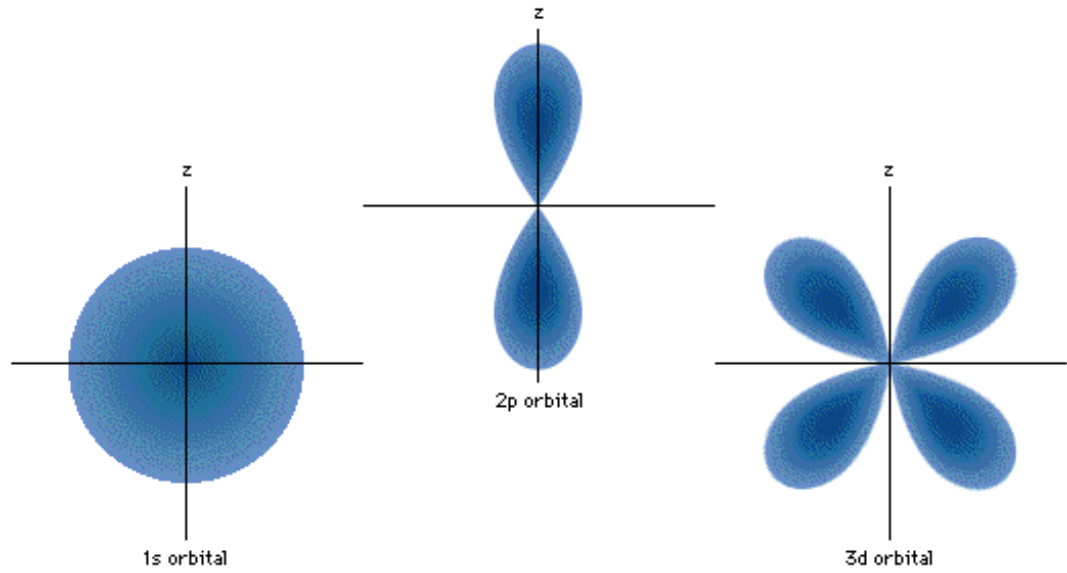
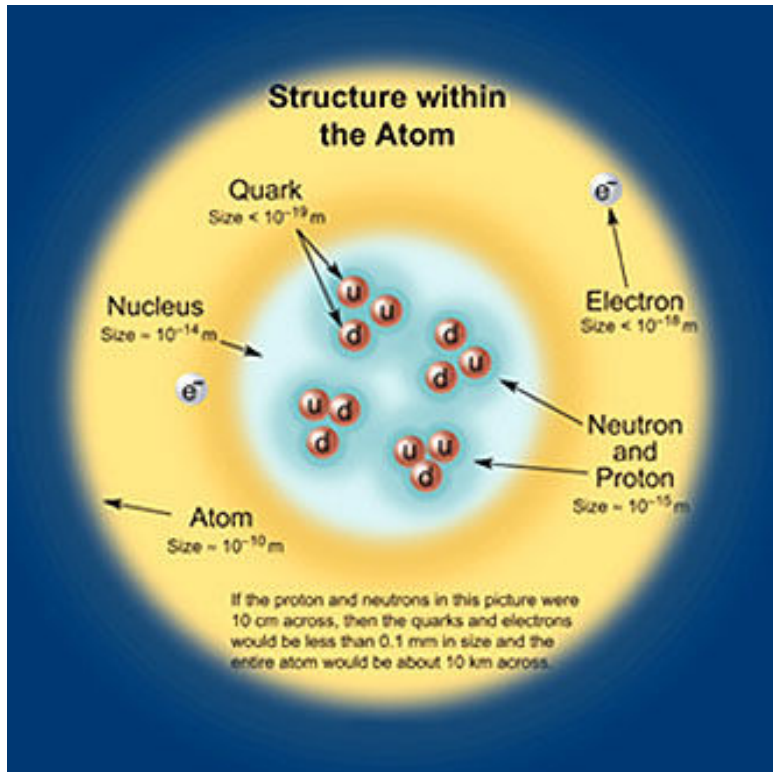
**Energy is conserved in core-level atomic transitions
(only induced by X-rays or Gamma rays)**



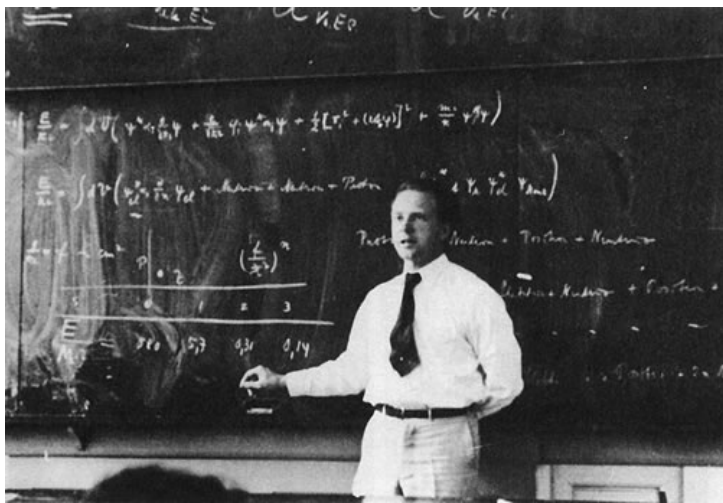
Remember: Electrons exist at discrete orbitals (Hence they have discrete absorption behavior of incoming X-rays)



Energy of ejected electrons (characteristic)



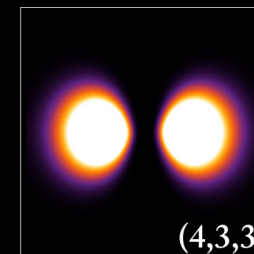
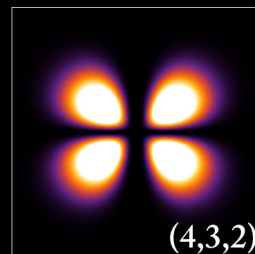
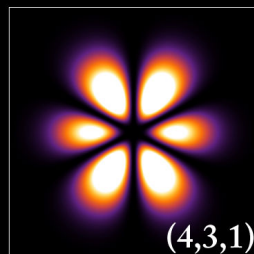
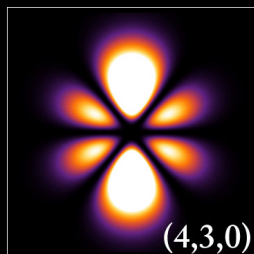
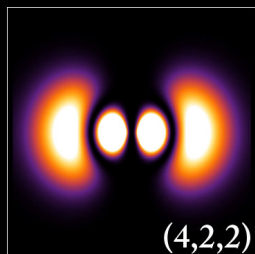
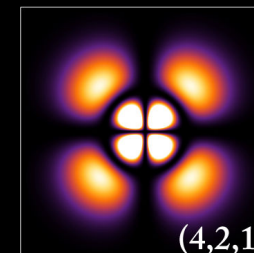
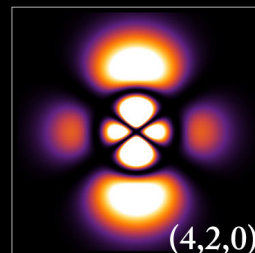
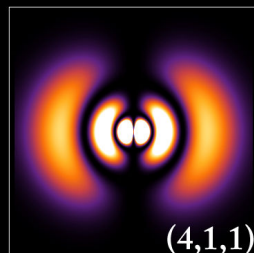
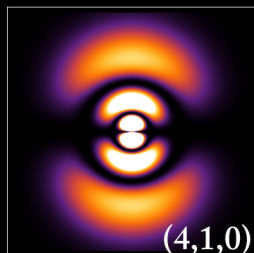
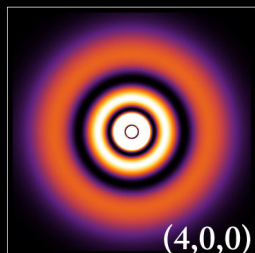
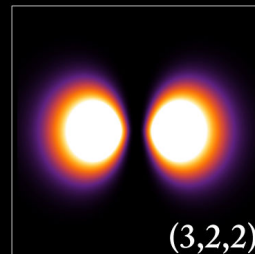
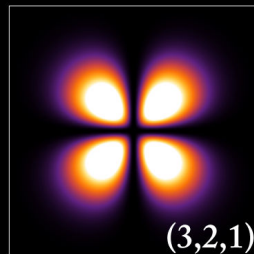
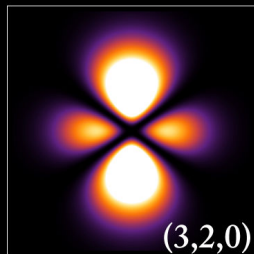
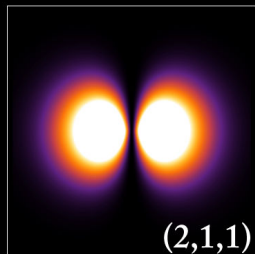
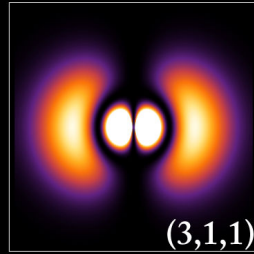
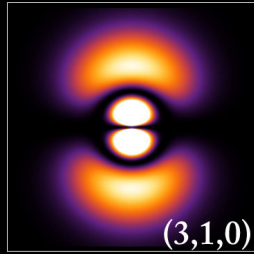
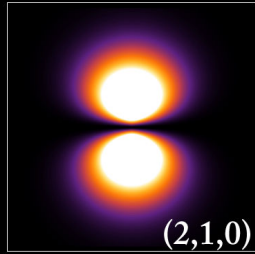
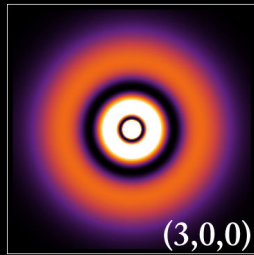
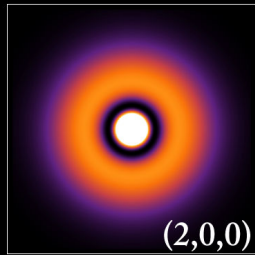
We cannot talk about well-defined discrete orbitals but rather probabilities of finding electrons at specific sites around the nucleus.



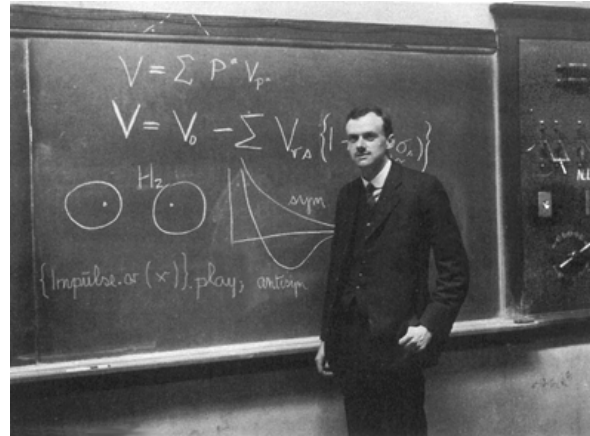
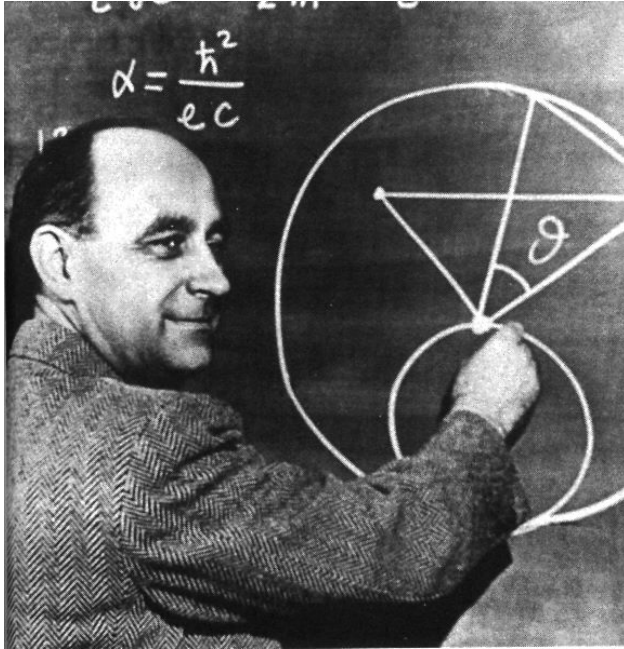
Hydrogen Wave Function

Probability density plots.

$$\psi_{nlm}(r, \vartheta, \varphi) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]}} e^{-\rho/2} \rho^l L_{n-l-1}^{2l+1}(\rho) \cdot Y_{lm}(\vartheta, \varphi)$$



Enrico Fermi and Paul Dirac developed an expression relating the temperature dependent distribution of electrons around nuclei:



Fermi-Dirac distribution of electrons in a crystal obey



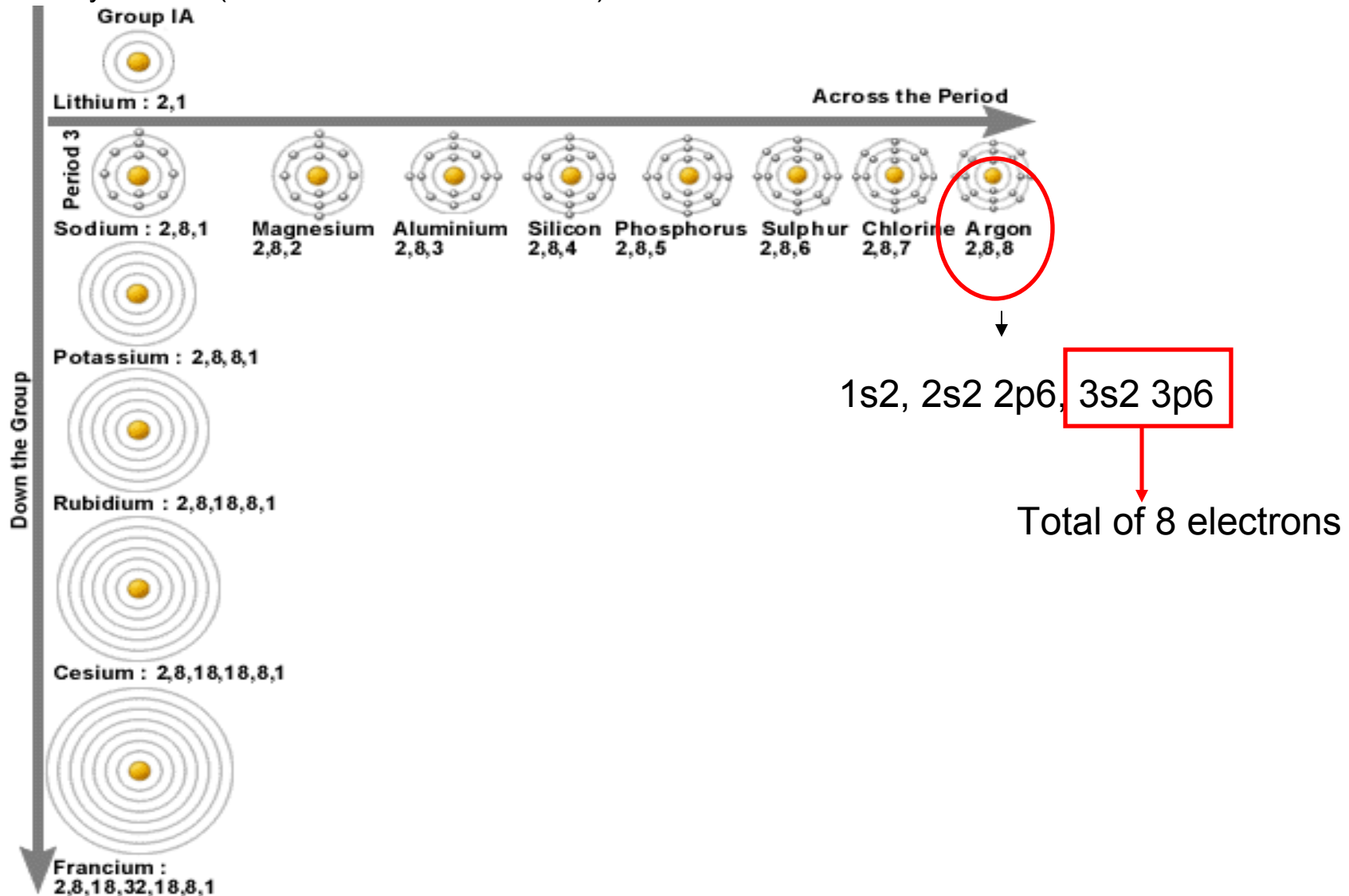
The Pauli principle !

What do all these things imply about our experience of everyday structures?

- Remember the fact about noble (inert) gases?

Inert gases form the simplest crystals for which:

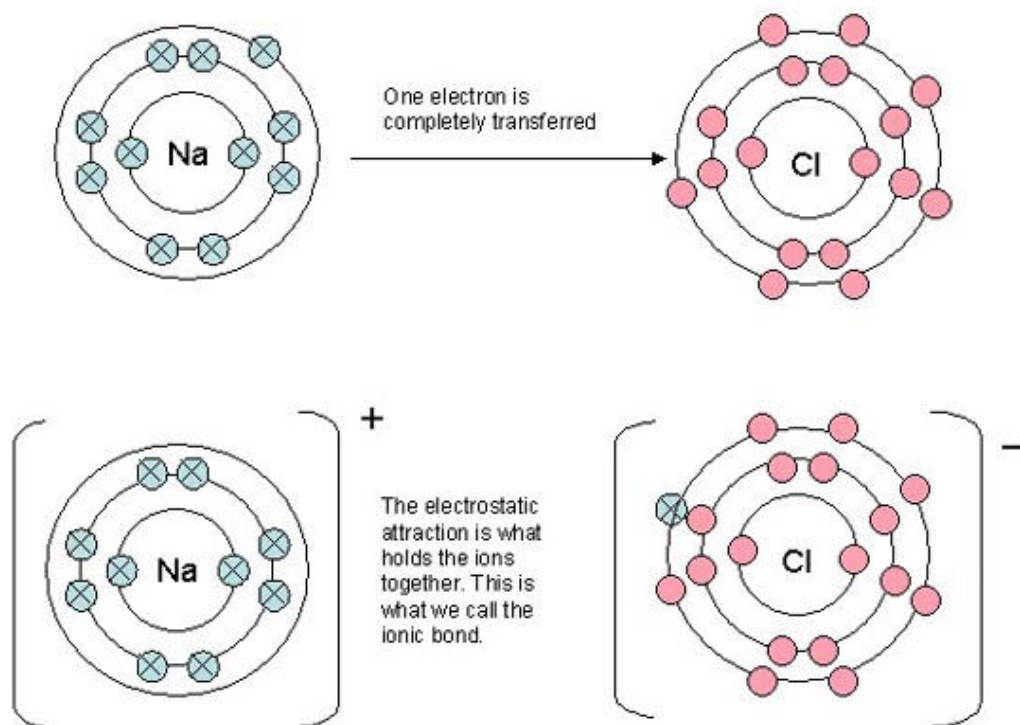
1. The electron distribution is very close to that of free atoms
2. The outermost electron shells are completely filled and the charge distribution is spherically symmetric (We will come to this later on)



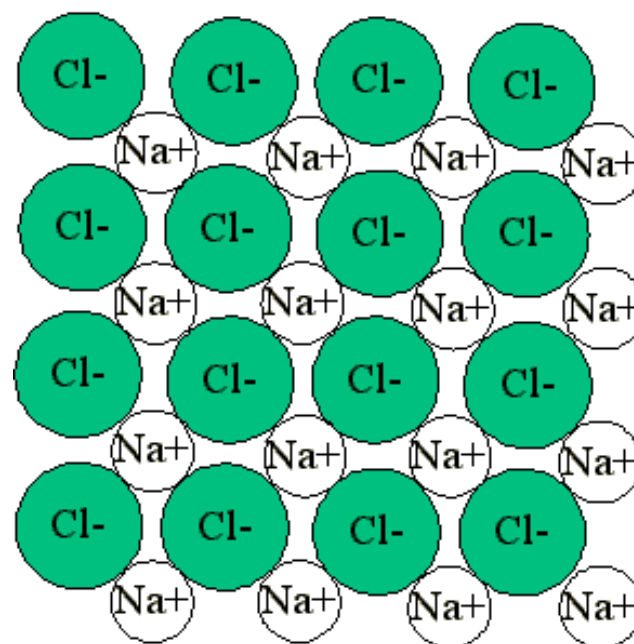
‘A stable compound occurs when the total energy of the combination has lower energy than the separated atoms.’ (www. hyperphysics.phy-astr.gsu.edu)

Note: All condensed matter is a result of the effect of Coulomb forces and electron configuration around the nuclei of individual atoms.

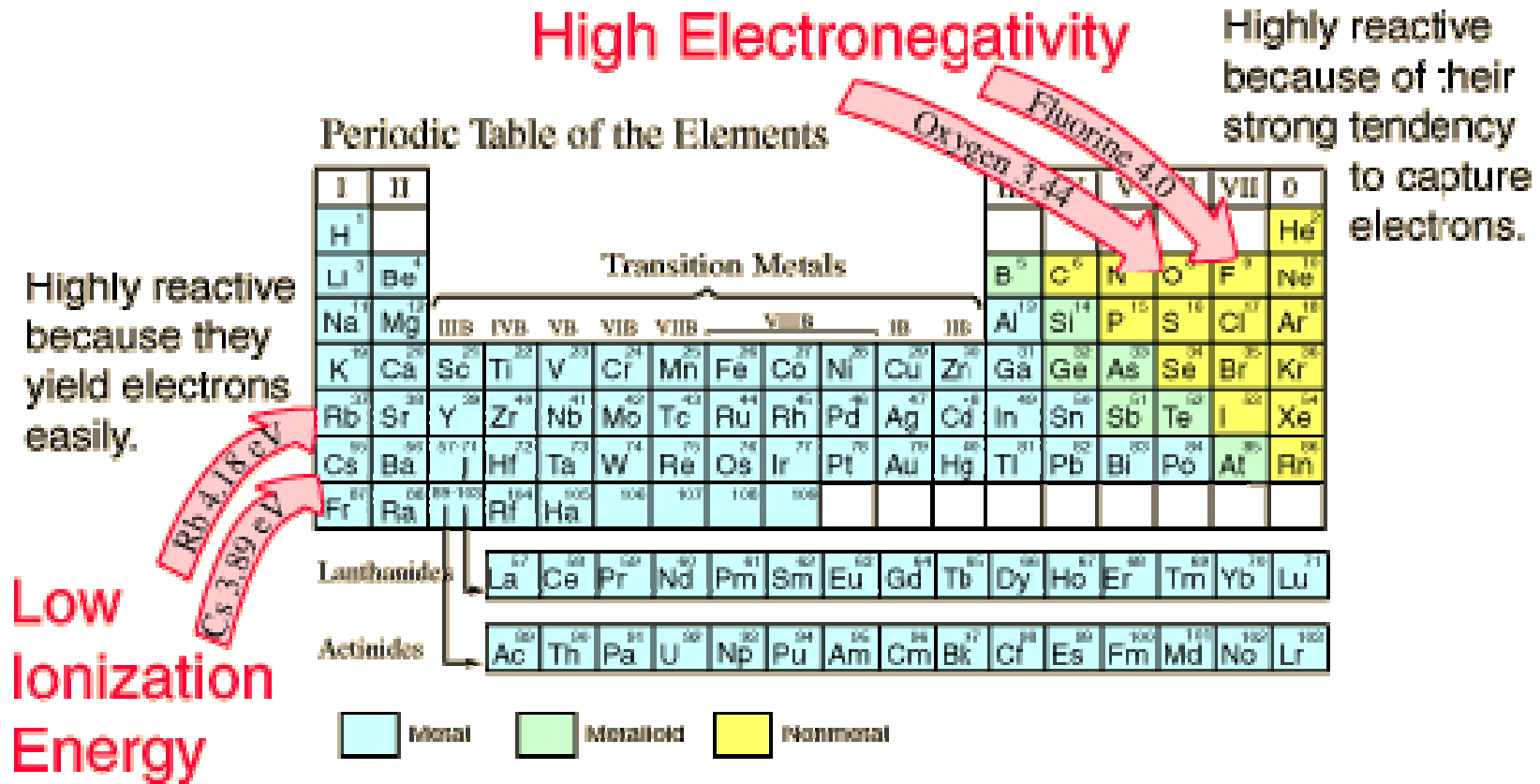
$$F = \frac{1}{4\pi\epsilon_0} \frac{q_1q_2}{r^2} \quad E = \frac{1}{4\pi\epsilon_0} \frac{q}{r^2}$$



Slice through a NaCl crystal

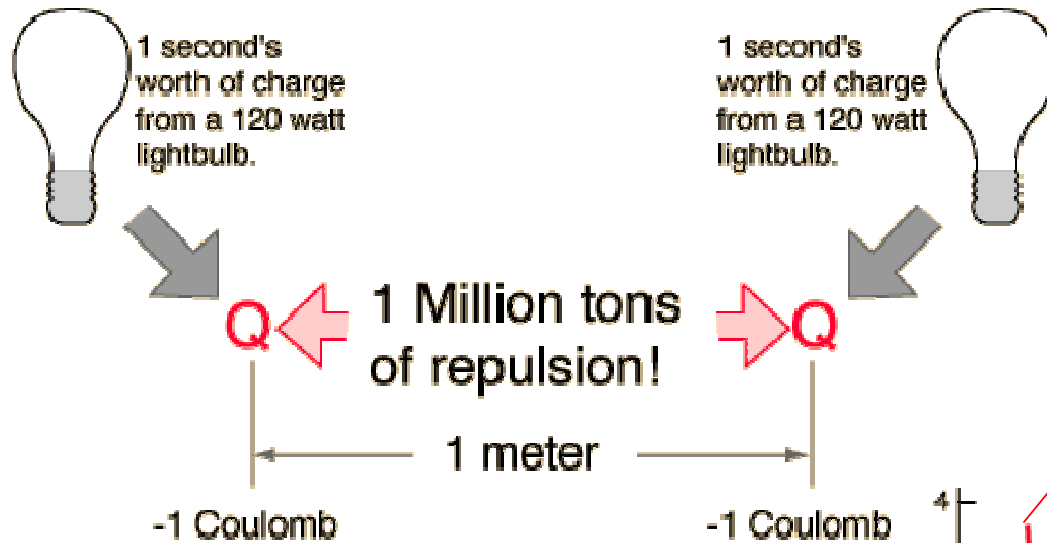


How does electronegativity and affinity come into play?



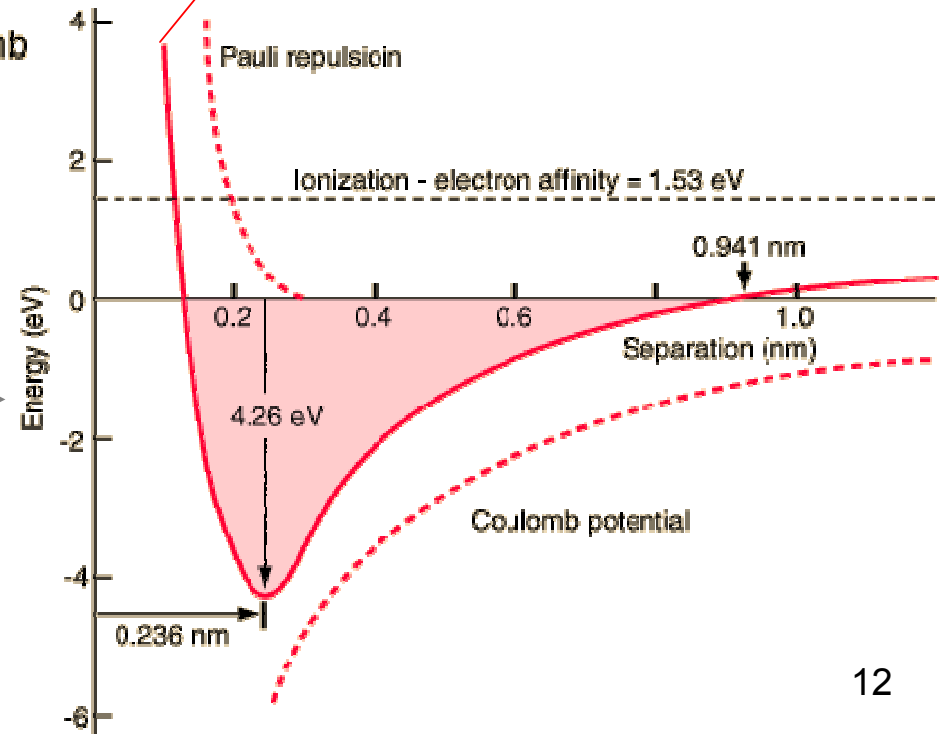
The highly reactive corners of the Periodic Table

Electrostatic forces are very strong:



Solid red curve
Pauli repulsion + Coulomb potential

For NaCl



When two ions approach each other too much, the Pauli repulsion dominates (Pauli repulsion has nothing to do with the electrostatic interaction).

In some materials and gas-phase simulations:

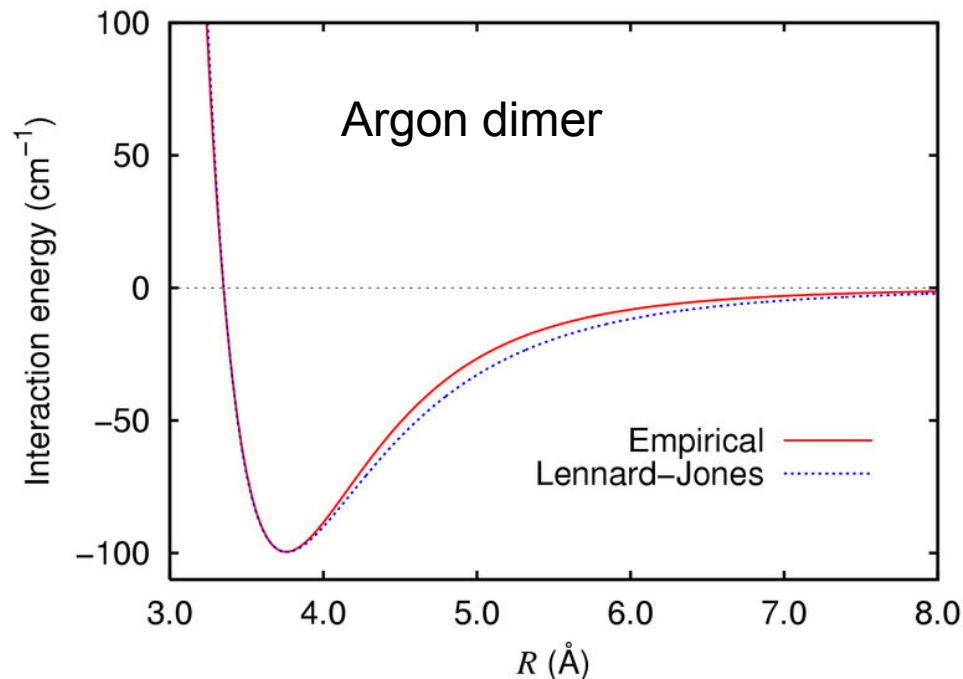
$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right]$$

Repulsive Attractive

Interaction potential (energy)
(Lenard-Jones potential)

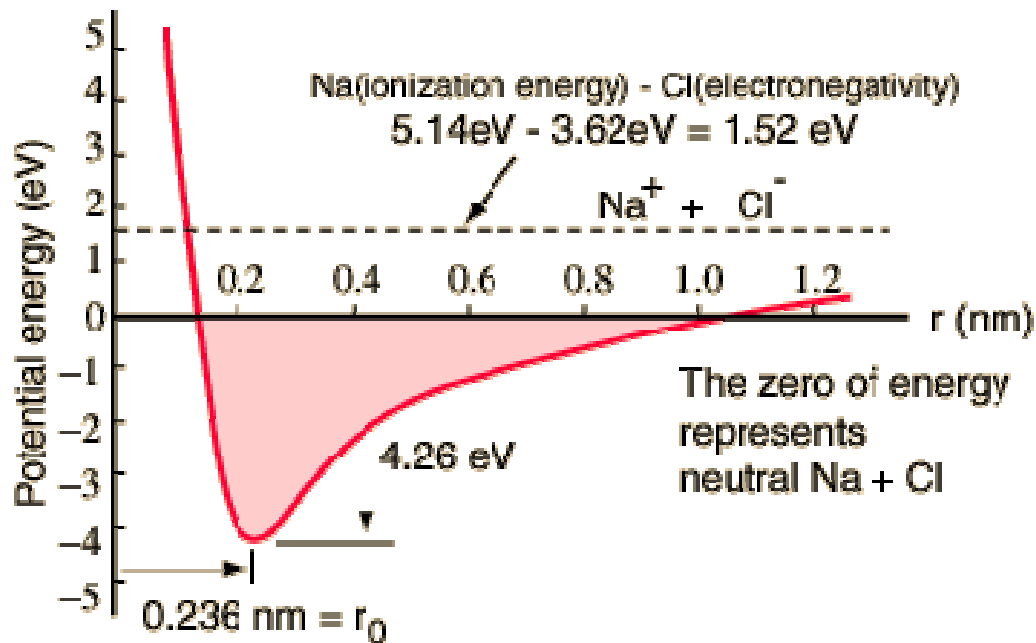
To find the equilibrium interatomic distance:

$$dV(r) / dr = 0$$



How does NaCl form? (Example to Coulomb force in action)

An atom of [sodium](#) has one 3s electron outside a closed shell, and it takes only 5.14 [electron volts](#) of energy to remove that electron. The [chlorine](#) lacks one electron to fill a shell, and releases 3.62 eV when it acquires that electron (it's [electron affinity](#) is 3.62 eV). This means that it takes only 1.52 eV of energy to donate one of the sodium electrons to chlorine when they are far apart. [When the resultant ions are brought closer together, their electric potential energy becomes more and more negative, reaching -1.52 eV at about 0.94 nm separation.](#) This means that if neutral sodium and chlorine atoms found themselves closer than 0.94 nm, it would be energetically favorable to transfer an electron from Na to Cl and form the ionic bond. (from <http://hyperphysics.phy-astr.gsu.edu>)



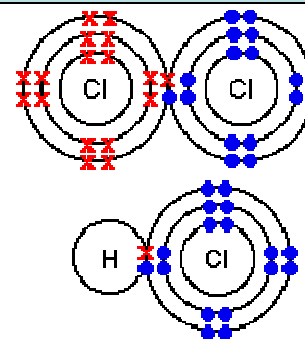
The driving force for formation of ionic bonds are fairly straightforward.

The tendency of an atom to form **covalent bonds** with other atoms is somewhat more involved to explain.

Single covalent bonds	Double covalent bonds
H-H	O=O
H-Cl	C=O
F-F	C=C
	And etc.

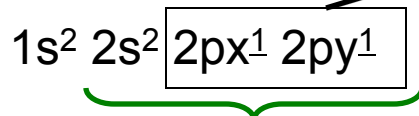
Electron cloud evenly distributed: Non-polar
(electronegativities nearly equal)

Electron cloud unevenly distributed: Polar
(electronegativities different)



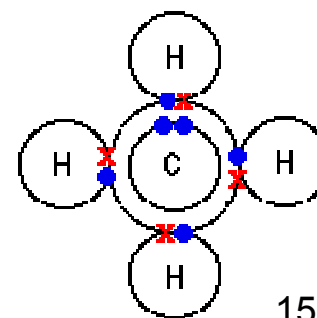
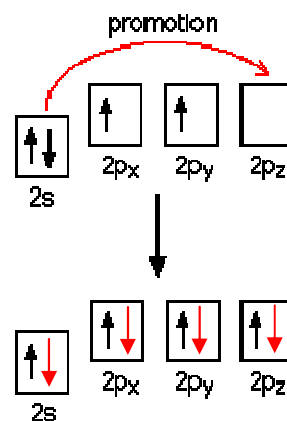
When an atom wants to have inert gas configuration for outer shell electrons, it will find a way....

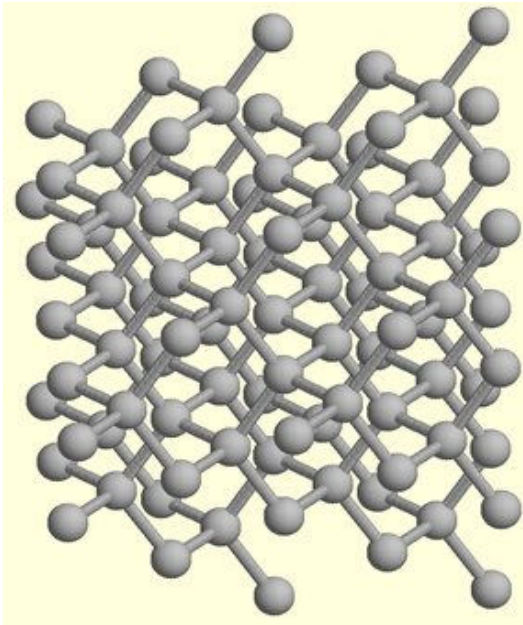
For Carbon in its ground state:



They have nearly the same energy electrons

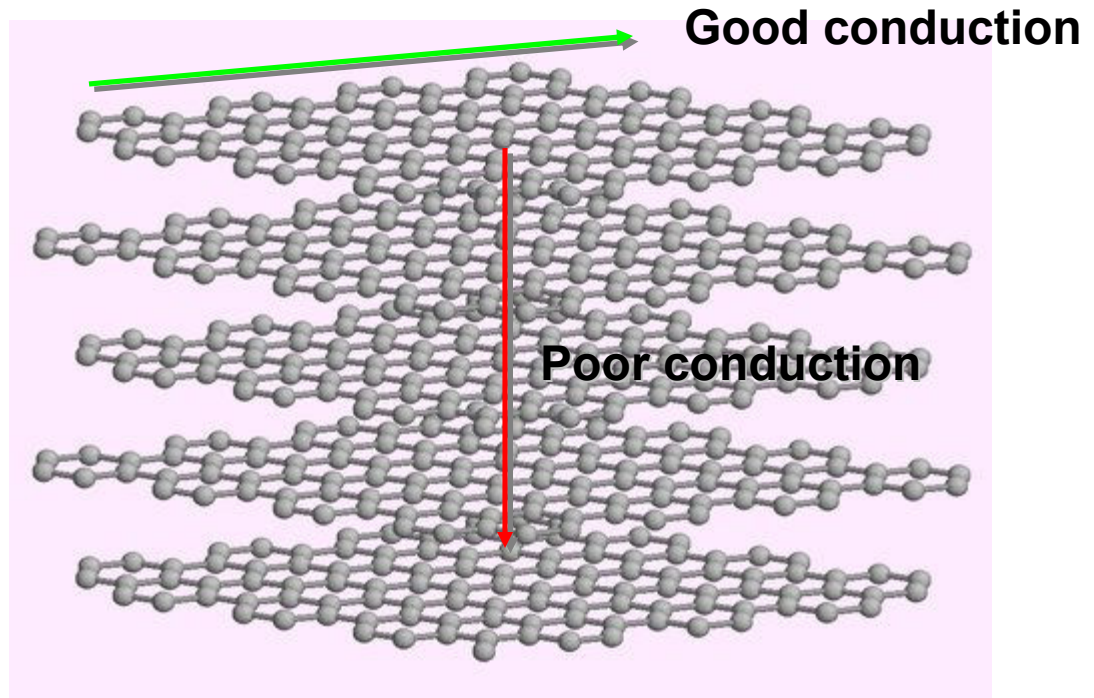
Why not CH_2 but CH_4 ?





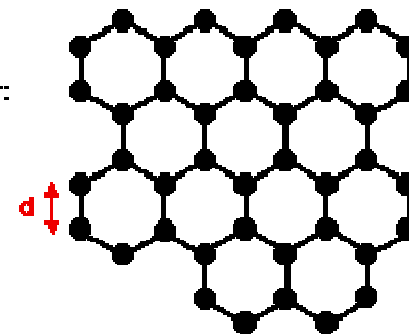
Carbon (Diamond: forms at high pressure and temperature)
Insulator phase

Conductivity: It is all about whether bonds enable delocalization of electrons or not.

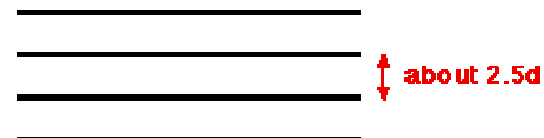


Carbon in graphite form (much more common than diamond and more stable)

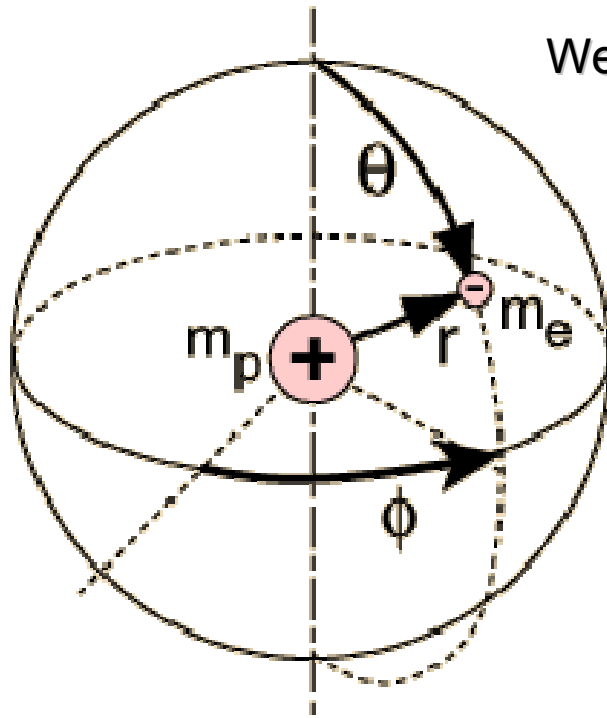
atoms in one layer:



a stack of layers:



Some helpful details about the quantum state concept



The electrostatic potential due to the nucleus is spherically symmetric.

We call this 'the quantum state' of a particle

$$\Psi(r, \theta, \phi) = R(r)P(\theta)F(\phi) \times \text{spin of electron } \left(\downarrow \text{ or } \uparrow \right)$$

n	ℓ	m_ℓ
principal quantum number	orbital quantum number	magnetic quantum number

$$U(r) = \frac{-e^2}{4\pi\epsilon_0 r}$$

Electrostatic potential energy of an electron in orbit at a distance r from the nucleus.

Pauli principle: No two fermions can exist in the same quantum state in a system.