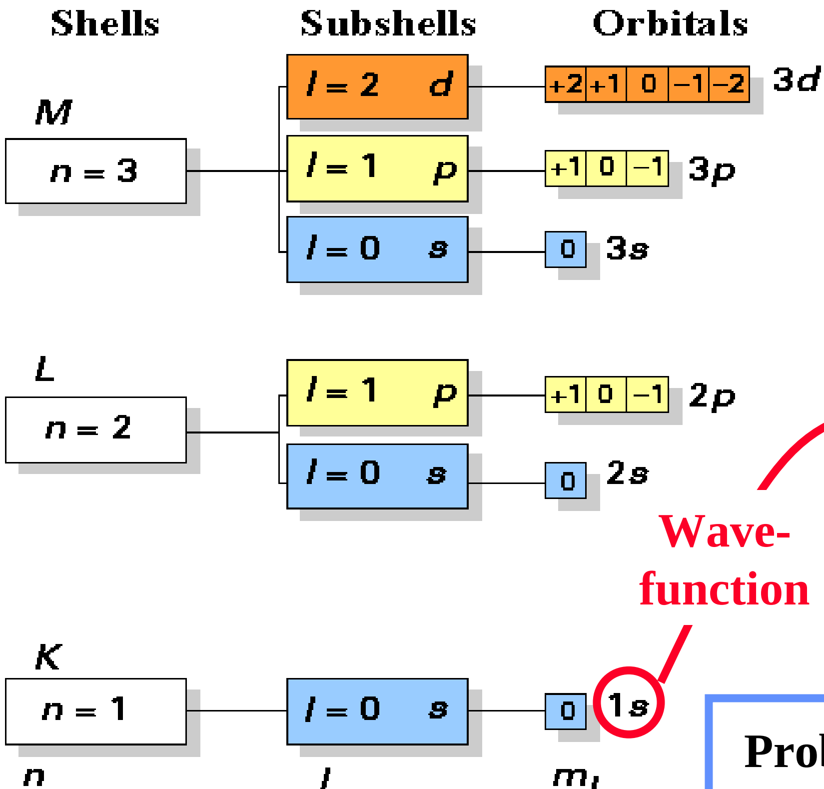
Orbitals and their Wavefunctions



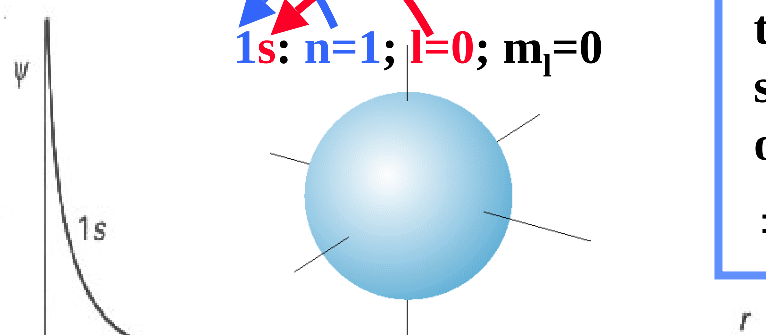
n^2 different orbitals

$$\Psi = \frac{1}{\sqrt{\pi a_0^{\,3}}} e^{-r/a_0}; \quad a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{m_e e^2}$$

Wave-function

Bohr radius a_0 = 52.9pm

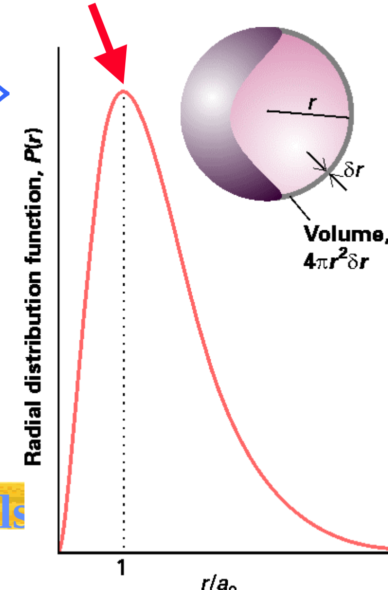
1s: n=1; l=0; m_l=0

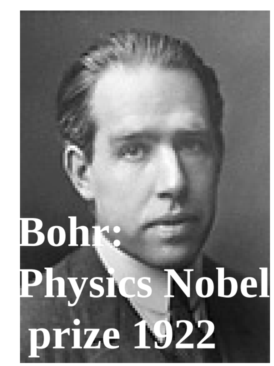


Probability to find electron between two spherical surfaces (area $4\pi r^2$) of thickness δr

$$= 4\pi r^2 \Psi^2 \delta r$$

$\Rightarrow$



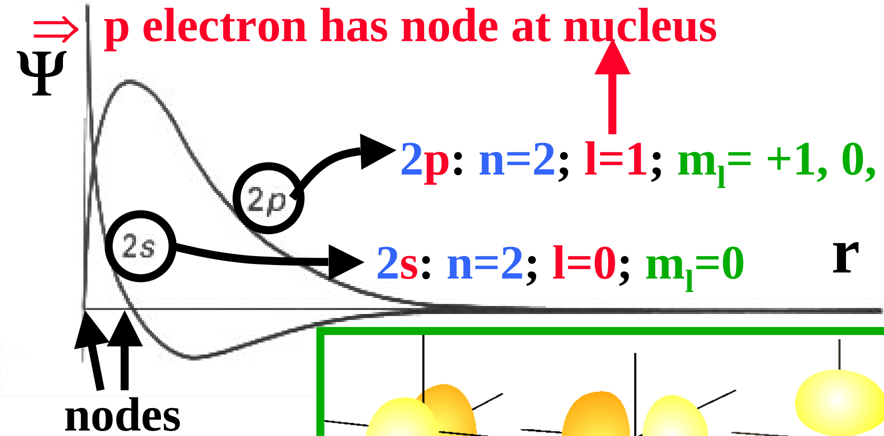


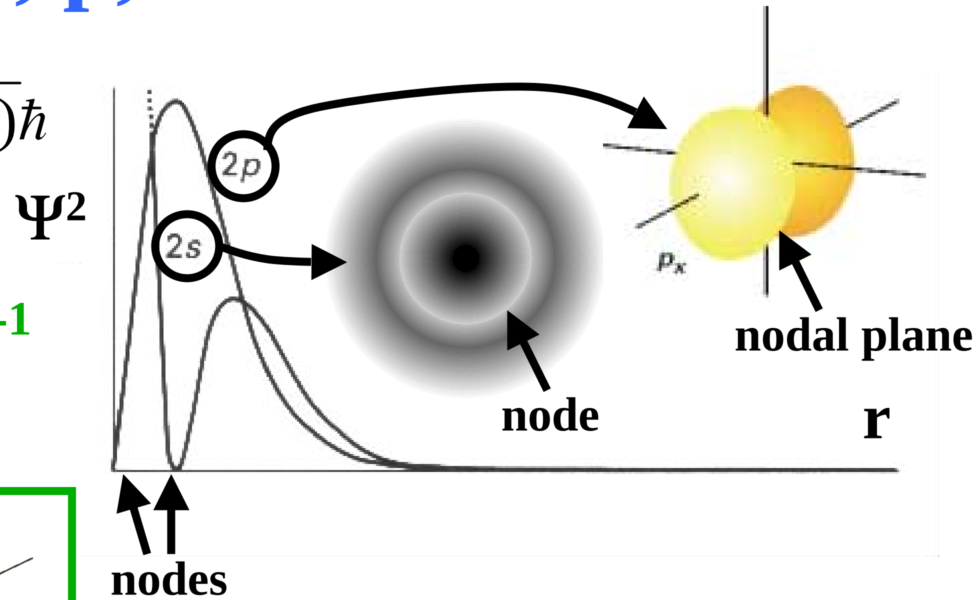
Boundary surface is spherically symmetric

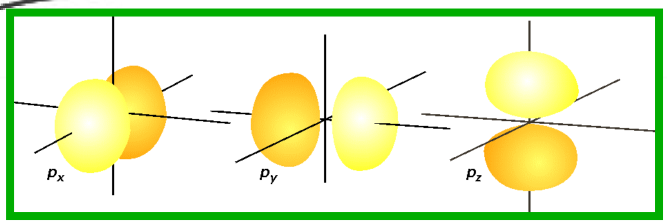
Wavefunctions: s, p, and d Orbitals

Quantized angular momentum $= \sqrt{l(l+1)}\hbar$

$\Rightarrow$ **p electron has node at nucleus**



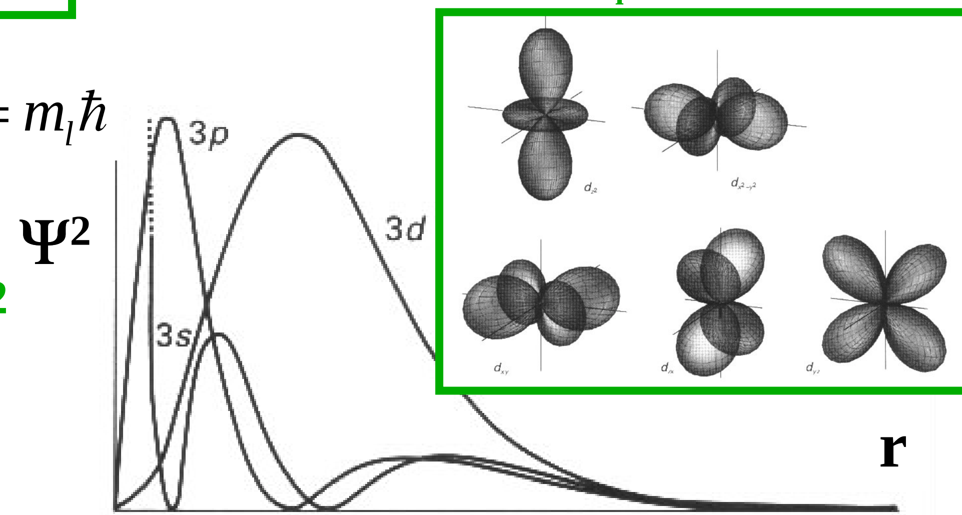


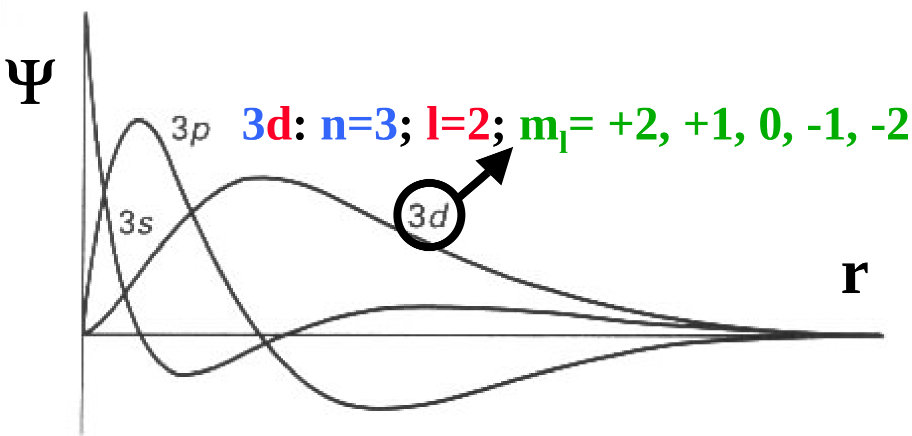


p orbitals: m_l= +1, 0, -1

z component of angular momentum $= m_l\hbar$

d orbitals: m_l= +2, +1, 0, -1, -2

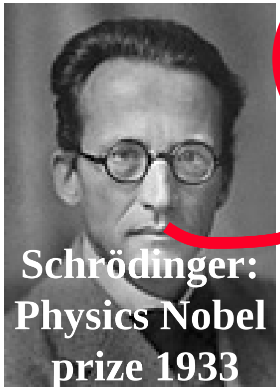




We Ain’t Seen Nothing Yet: Many-Electron Atoms

What about atoms with 2 electrons such as He?

Each electron will influence all others!



Schrödinger: Physics Nobel prize 1933

?!

⇒ No analytical, only numerical solutions with some “cheating”

⇒ Orbital approximation: Each electron occupies an independent orbital, e.g., in He :

$$\Psi = \Psi(1) \times \Psi(2) = \sqrt{\frac{8}{\pi a_0^3}} e^{-2r_1/a_0} \times \sqrt{\frac{8}{\pi a_0^3}} e^{-2r_2/a_0} = \left(\frac{8}{\pi a_0^3}\right) e^{-2(r_2+r_2)/a_0}$$

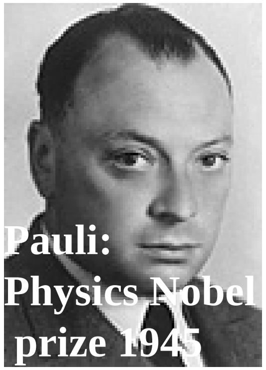
Overall wavefunction

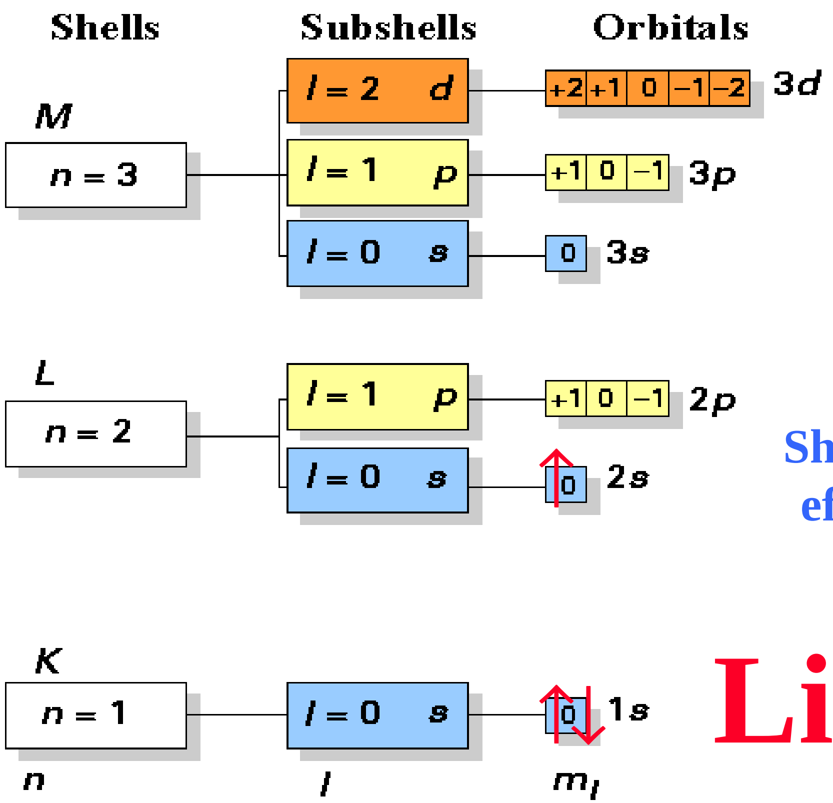
“Configuration” = list of occupied orbitals: H = $1s^1$; He = $1s^2$

Li has three electrons with configuration $1s^2 2s^1$ = [He]$2s^1$; Why?

More and More Electrons

Pauli Exclusion principle: No more than 2 electrons may occupy the same orbital; if they do their electrons have to be paired: ↑↓, i.e., one electron is $m_s = +1/2$, one $-1/2$

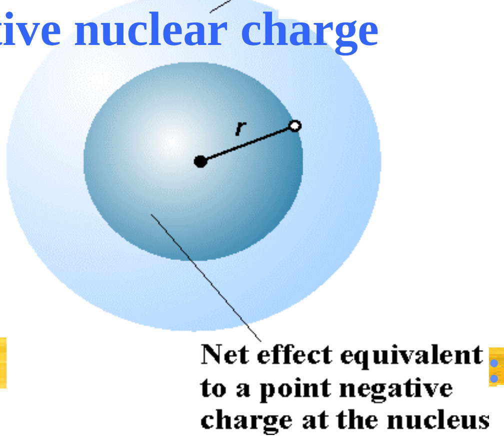




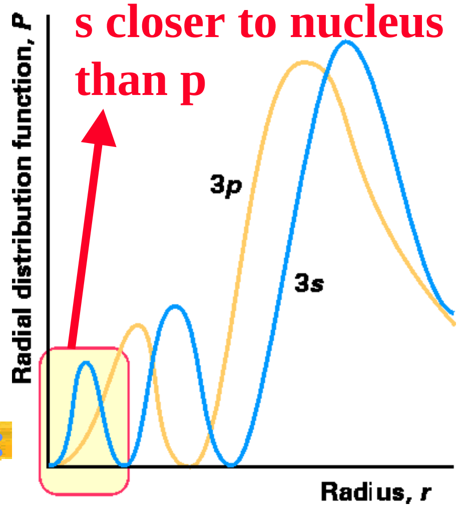
Li

In many-electron atoms orbitals of the same shell are no longer degenerate, i.e., energies: s<p<d<f, due to their different shielding from the nucleus

Shielding leads to a lower effective nuclear charge

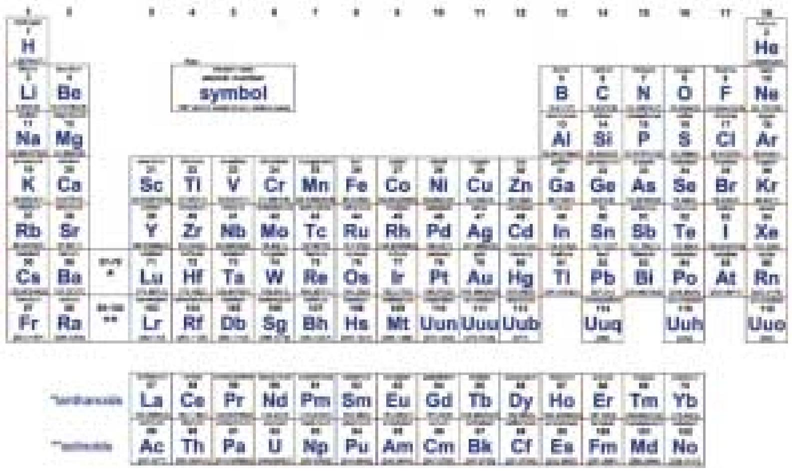


s closer to nucleus than p



Rules for Building up Higher Elements

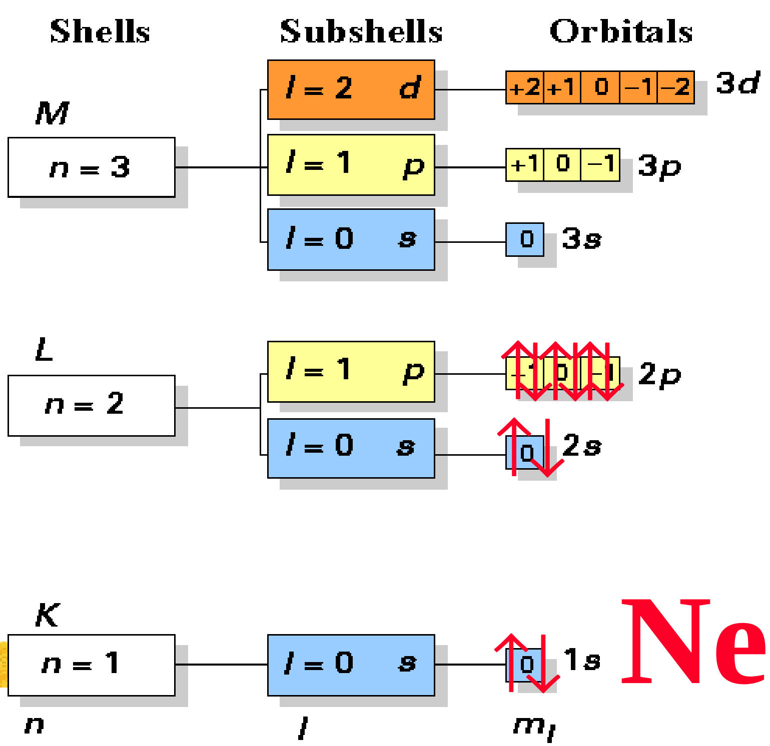
1.) Order of orbital occupation: 1s 2s 2p 3s 3p 4s 3d 4p 5s 4d 5p 6s 5d 4f 6p...



2.) **Pauli exclusion principle:**
2 electrons/orbital

3.) Electrons occupy different orbitals of a given subshell before doubly occupying any one of them

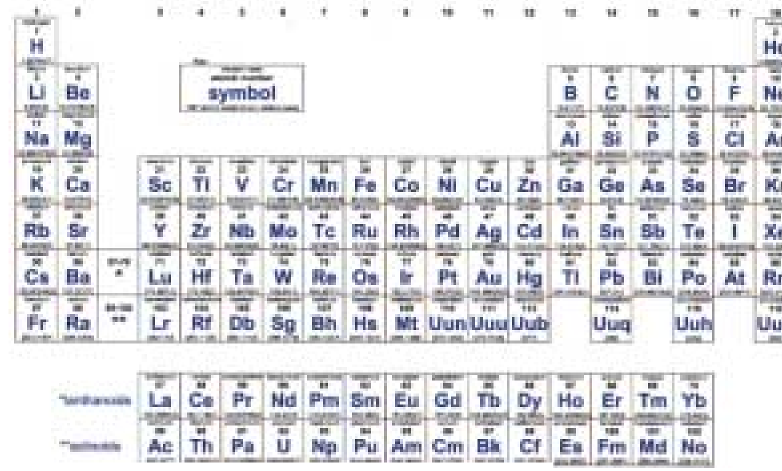
4.) **Hund's rule:**
In its ground state, an atom adopts a configuration with the greatest number of unpaired electrons

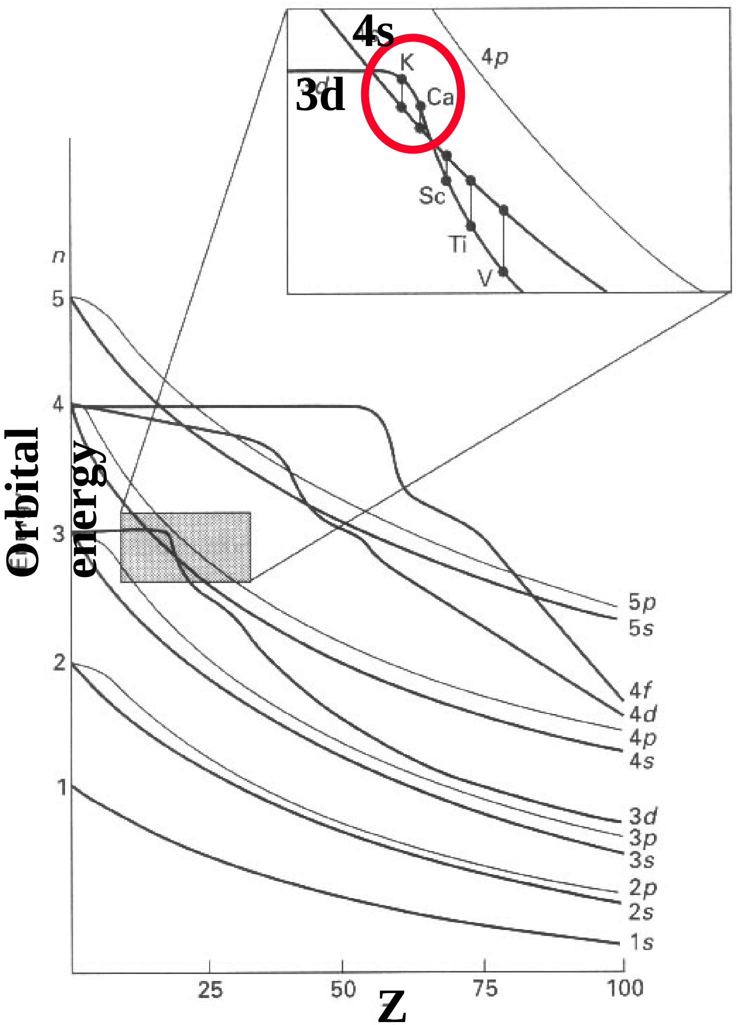


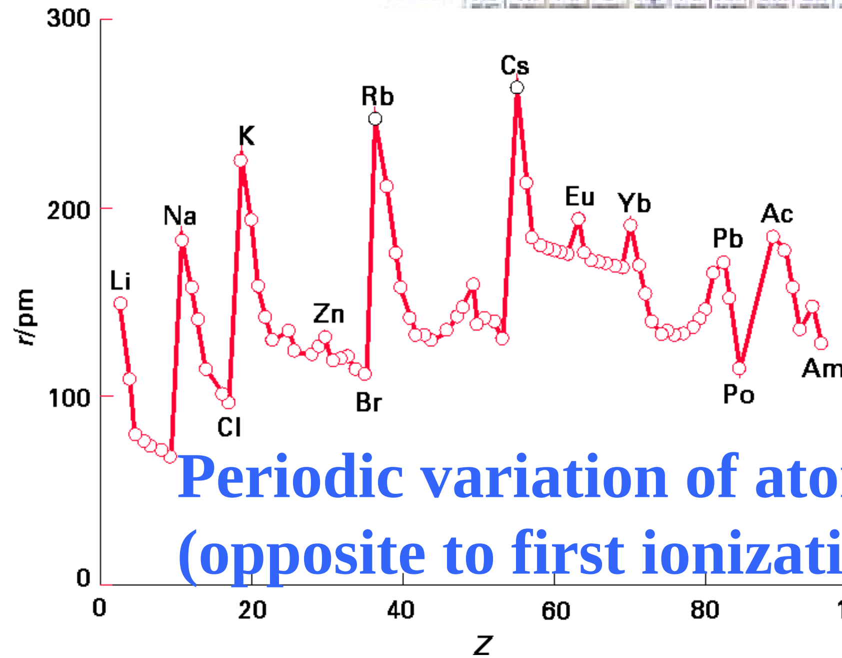
Ne

The Periodic Table of the Elements

Order of orbital occupation: 1s 2s 2p 3s 3p 4s 3d 4p 5s 4d 5p 6s 5d 4f 6p...







Periodic variation of atomic radius (opposite to first ionization energy)