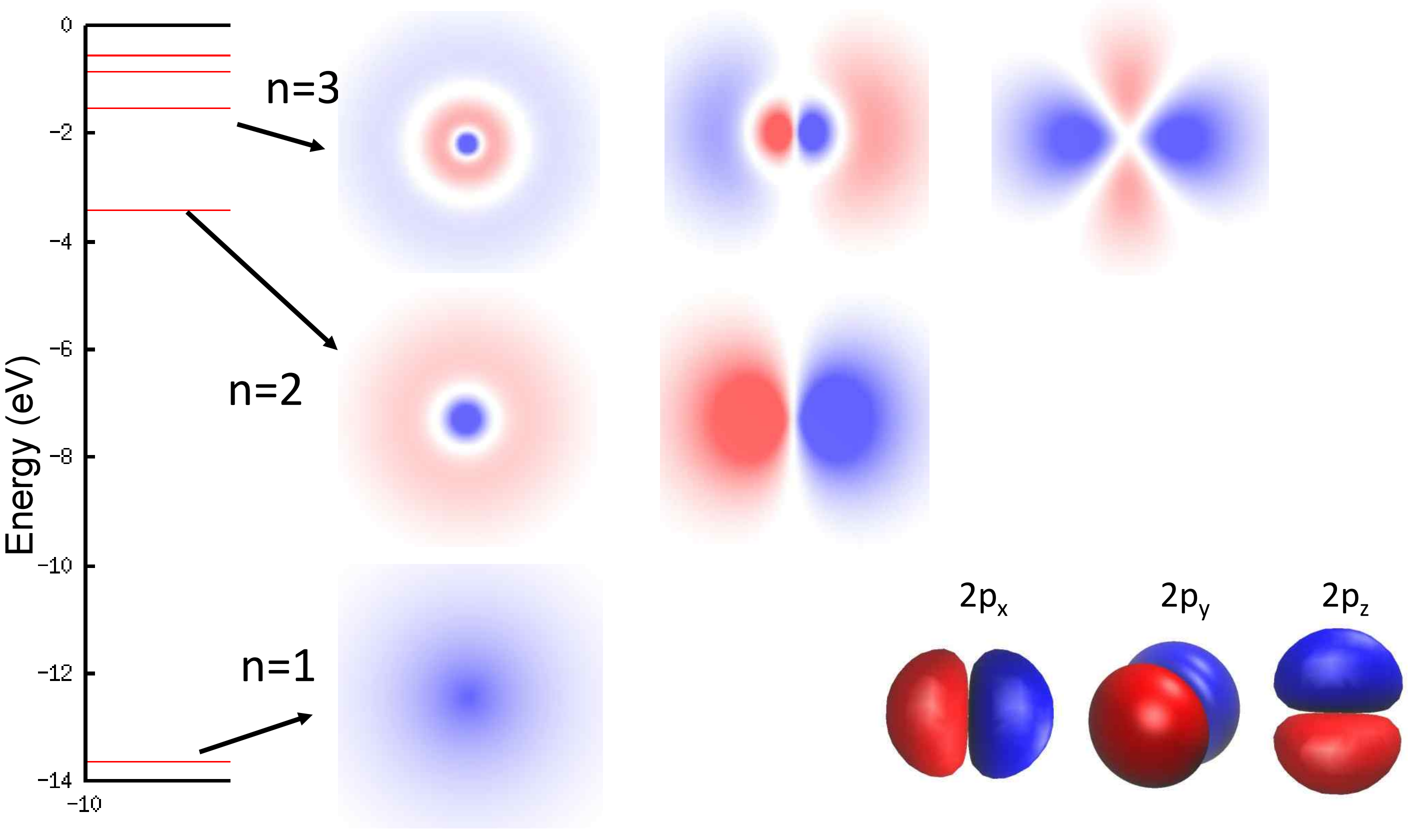
Part 1: bonding

- Why we need Quantum Mechanics?
  - The hydrogen atom
- Basic Quantum Mechanics
  - Schrodinger equation and simple solutions
- Electronic structure of atoms
  - Hydrogen and multi-electron atoms
- Bonding in molecules
  - The simplest molecule H2+
  - First row hydrides
  - Covalent, ionic and van der Waals interactions
- Bonding in crystalline solids
  - Band structure
  - Covalent vs. metallic bonding

Hydrogen excited states



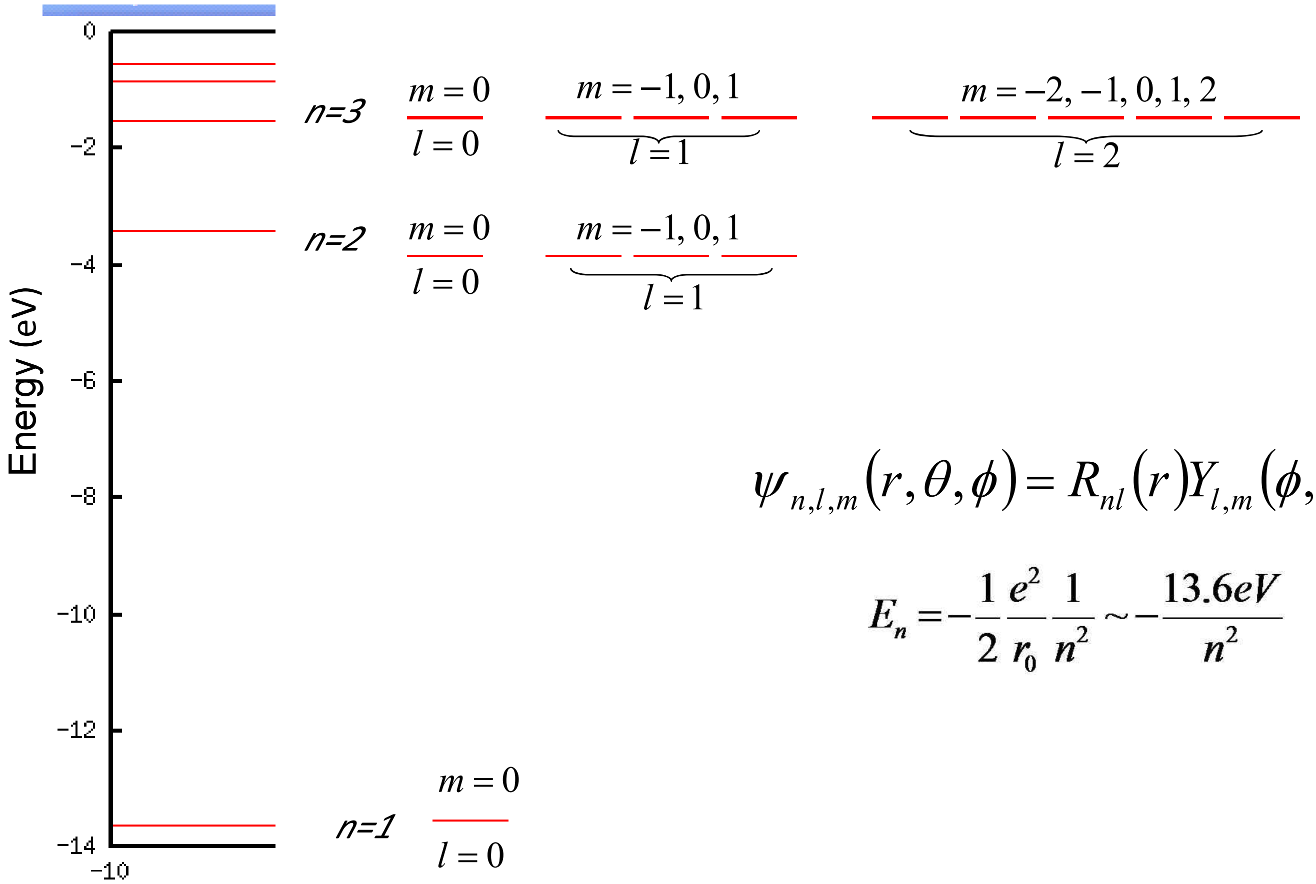
Hydrogen general solution

$$\psi_{n,l,m}(r,\theta,\phi) = R_{nl}(r) Y_{l,m}(\phi,\theta)$$

Three quantum numbers

- *n* principal quantum number
  - Energy depends on n: $E_n = -\frac{13.6eV}{n^2} Z^2$
- *l* angular momentum quantum number
  - Values limited by principal quantum number: 0, 1, …, *n*-1
- *m* magnetic quantum number (projection of *l* along z axis)
  - Values limited by *l*: *m*=-*l*, -*l*+1, …,*l*-1, *l*

Summary: hydrogen solution



$$\psi_{n,l,m}(r,\theta,\phi) = R_{nl}(r) Y_{l,m}(\phi,\theta)$$

$$E_n = -\frac{1}{2}\frac{e^2}{r_0}\frac{1}{n^2} \sim -\frac{13.6eV}{n^2}$$

Wavefunctions

Table 3.1. *States of one-electron atoms*

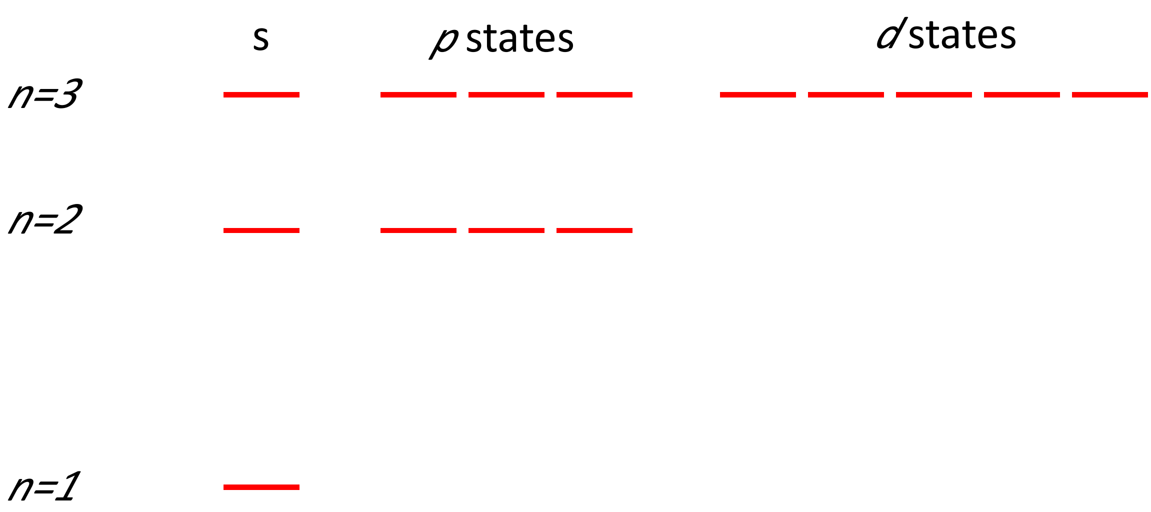
n	l	$\lvert m \rvert$	Spectroscopic designation	E_n in units of $e^2/2a_0$	g	$\psi_{n,l,m}(r,\theta,\phi)$
1	0	0	1s	-1	1	$N_1 \exp(-Zr/a_0)$
2	0	0	2s	$-\frac{1}{4}$		$N_2(2 - Zr/a_0)\exp(-Zr/2a_0)$
2	1	0	$2p_z$	$-\frac{1}{4}$	4	$N_2(Zr/a_0)\exp(-Zr/2a_0)\cos\theta$
2	1	1, cos	$2p_x$	$-\frac{1}{4}$		$N_2(Zr/a_0)\exp(-Zr/2a_0)\sin\theta\cos\phi$
2	1	1, sin	$2p_y$	$-\frac{1}{4}$		$N_2(Zr/a_0)\exp(-Zr/2a_0)\sin\theta\sin\phi$
3	0	0	3s	$-\frac{1}{9}$		$N_3[27 - 18(Zr/a_0) + 2(Zr/a_0)^2]\exp(-Zr/3a_0)$
3	1	0	$3p_z$	$-\frac{1}{9}$		$N_3\sqrt{6}\,(6 - Zr/a_0)(Zr/a_0)\exp(-Zr/3a_0)\cos\theta$
3	1	1, cos	$3p_x$	$-\frac{1}{9}$		$N_3\sqrt{6}\,(6 - Zr/a_0)(Zr/a_0)\exp(-Zr/3a_0)\sin\theta\cos\phi$
3	1	1, sin	$3p_y$	$-\frac{1}{9}$	9	$N_3\sqrt{6}\,(6 - Zr/a_0)(Zr/a_0)\exp(-Zr/3a_0)\sin\theta\sin\phi$
3	2	0	$3d_{3z^2-r^2}$	$-\frac{1}{9}$		$N_3\sqrt{1/2}(Zr/a_0)^2\exp(-Zr/3a_0)(3\cos^2\theta - 1)$
3	2	1, cos	$3d_{xz}$	$-\frac{1}{9}$		$N_3\sqrt{6}(Zr/a_0)^2\exp(-Zr/3a_0)\sin\theta\cos\theta\cos\phi$
3	2	1, sin	$3d_{zy}$	$-\frac{1}{9}$		$N_3\sqrt{6}(Zr/a_0)^2\exp(-Zr/3a_0)\sin\theta\cos\theta\sin\phi$
3	2	2, cos	$3d_{x^2-y^2}$	$-\frac{1}{9}$		$N_3\sqrt{3/2}(Zr/a_0)^2\exp(-Zr/3a_0)\sin^2\theta\cos 2\phi$
3	2	2, sin	$3d_{xy}$	$-\frac{1}{9}$		$N_3\sqrt{3/2}(Zr/a_0)^2\exp(-Zr/3a_0)\sin^2\theta\sin 2\phi$

$$N_1 = \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2}, \quad N_2 = \frac{1}{4}\left(\frac{Z^3}{2\pi a_0^3}\right)^{1/2}, \quad N_3 = \frac{1}{81}\left(\frac{Z^3}{3\pi a_0^3}\right)^{1/2}$$

Martin Karplus and Richard N. Porter
Atoms and molecules: an introduction for students of physical chemistry

Atoms with multiple electrons

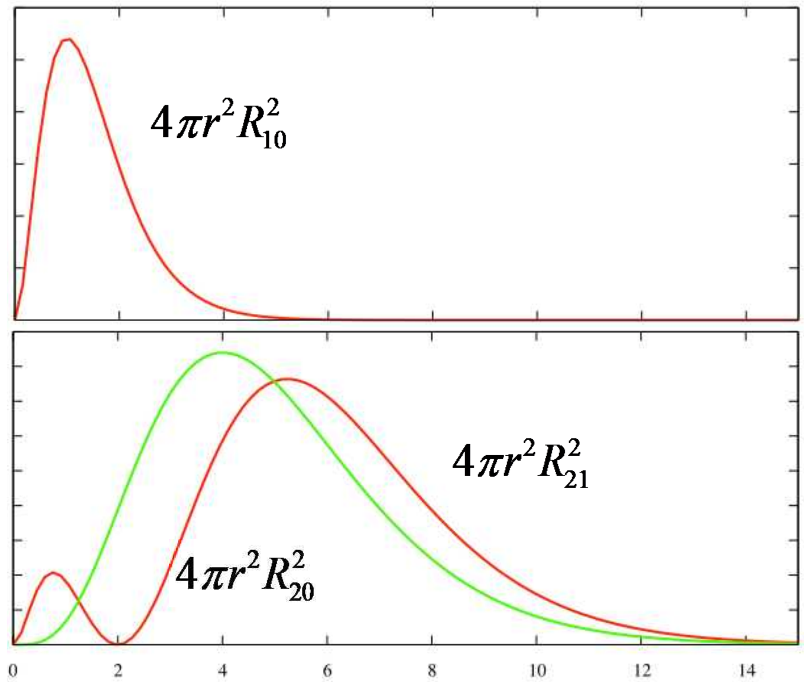
- Orbitals maintain the shape of hydrogen ones
- We'll use hydrogen-like orbitals for other atoms



Lithium and shielding

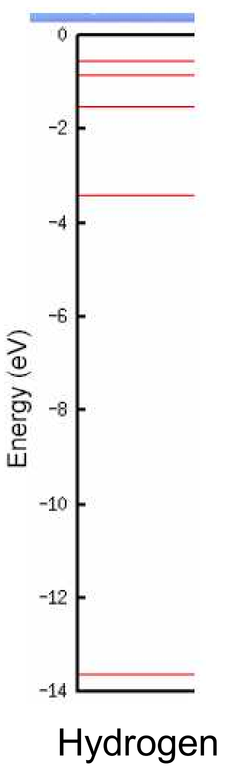
•Electrons in inner shells shield the nuclear potential to outer electrons

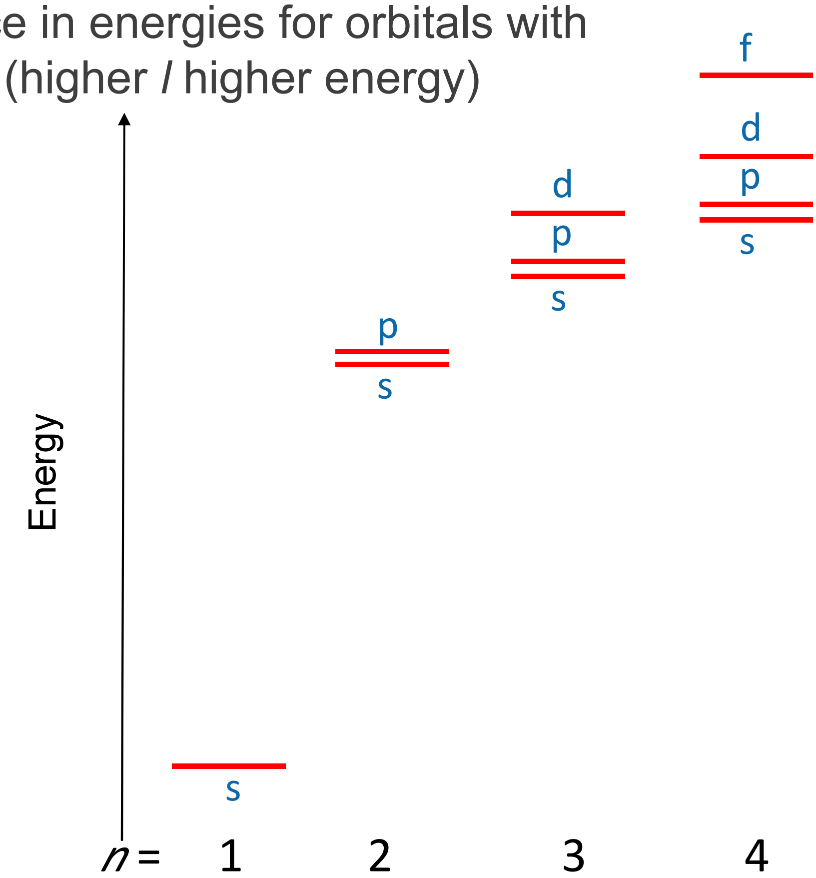
- •Energy depends not only on n, but also on *l*
- •The larger the angular momentum number l, the higher the energy



Energy levels

•Shielding cause difference in energies for orbitals with the same *n* and different *l* (higher *l* higher energy)





Hund’s rule and exchange interaction

	1s	2s	2p		
H					
He					
Li	↑↓				
Be	↑↓				
B	↑↓	↑↓			
C	↑↓	↑↓			
N	↑↓	↑↓			
O	↑↓	↑↓			
F	↑↓	↑↓			
Ne	↑↓	↑↓			

How do we fill orbitals?

Hund’ s rule:

All orbitals with a given *l* have to be filled with e- with the same spin first