

(4) Today

2.2.2 Quantum Numbers and Atomic Wave Functions

2.2.3 The Aufbau Principle

2.2.4 Shielding

(6) Second Class from Today

2.3 Periodic Properties

3.1 Lewis Structures

3.2 VSEPR

Next Class (5)

2.3 Periodic Properties

Third Class from Today (7)

3.2 VSEPR

Orbitals and Quantum Numbers (n, l, and m_l)

One quantum number wasn't enough to model the electrons in an atom

n is the principal quantum number

allowed values are the whole numbers starting a 1

l is the Angular momentum quantum number

allowed values are the from *n* to 0 in whole number increments

m_l is the magnetic quantum number

allowed values are the from -*l* to *l* in whole number increments

m_s is the spin quantum number

allowed values are - 1/2 or +1/2

e⁻ *n*=1 *l*=0 ~~*l*=1~~
e⁻ *n*=2 *l*=0
n=2 *l*=1

n=1 *l*=0 *m_l*=0

an *e*⁻ in the *n*=2 shell could have these allowed values

{	<i>n</i> =2	<i>l</i> =1	<i>m_l</i> =1
	<i>n</i> =2	<i>l</i> =1	<i>m_l</i> =0
	<i>n</i> =2	<i>l</i> =1	<i>m_l</i> =-1

↑ principal energy level ↑ orbital type ↑ 3 orbitals with *l*=1 shape that point in dif directions²

e⁻ *n*=2 *l*=1 *m_l*=0 *m_s*=+1/2
 2*p* *e*⁻ *l*=0 *s*
l=1 *p*
l=2 *d*
l=3 *f*

The angular distribution function:

The square of the angular distribution function describes the probability of finding the electron at angles θ and ϕ . In other words, picture yourself standing on the nucleus, and the electrons look like fog around you. The square of the angular distribution function describes how thick fog is when you look in different directions.

The Angular distribution function describes the basic shape of the orbital, or the number of lobes in an orbital. The angular distribution functions depend only on the quantum numbers l and m_l . That is, the angular distribution functions of all electrons with the same l and m_l values are the same regardless of n or m_s . Another way of saying this is that all s orbitals have the same basic shape. For example The 2s orbital ($n = 2, l = 0, m_l = 0$), the 3s ($n = 3, l = 0, m_l = 0$) and the 4s ($n = 4, l = 0, m_l = 0$) have the same basic shape (spherical)

The radial distribution function:

The square of the radial distribution function describes the probability of finding an a electron a given distance from the nucleus.

In other words, it tells you how far a way the fog starts to taper off, and it tell you whether or not there are pockets of clear sky in the fog.

The radial distribution function describes how far away from the nucleus the orbital extends and the number of nodes the orbital has.

The radial distribution functions depend on **both** n and l . This means that the number of nodes an orbital has and how far that orbital extends from the nucleus depends on the principle quantum number or energy level of the orbital (the **1** in **1s**, the **2** in **2s**, the **3** in **3s**, etc.) and the type of orbital (s vs. p vs. d).

Quantum Numbers	Angular Distribution Function	Radial Distribution Function
1s $n = 1, \ell = 0$	$\chi(s) = \left(\frac{1}{4\pi}\right)^{\frac{1}{2}}$	$R(1s) = 2 \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-\frac{\sigma}{a_0}}$ probability of finding e^- goes to 0 when $\sigma = 2$
2s $n = 2, \ell = 0$	$\chi(s) = \left(\frac{1}{4\pi}\right)^{\frac{1}{2}}$	$R(2s) = \frac{1}{2\sqrt{2}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} (2 - \sigma) e^{-\frac{\sigma}{2}}$ when $\sigma = 2$
3s $n = 3, \ell = 0$	$\chi(s) = \left(\frac{1}{4\pi}\right)^{\frac{1}{2}}$	$R(3s) = \frac{2}{81\sqrt{3}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} (27 - 18\sigma + 2\sigma^2) e^{-\frac{\sigma}{3}}$ two places where probability goes to 0
$n = 2, \ell = 1$	$\chi(P_x) = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}} \sin \theta \cdot \cos \phi$ $\chi(P_y) = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}} \sin \theta \cdot \sin \phi$ $\chi(P_z) = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}} \cos \theta$	$R(2p) = \frac{1}{2\sqrt{6}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \sigma e^{-\frac{\sigma}{2}}$ change in exponent shows e^- density falls off more slowly as one moves away from nucleus: 3 vs 2

$$\sigma = Zr/a_0$$

$$a_0 = \epsilon_0 h^2 / (\pi e^2 m_e)$$

3
l=0

p
l=1

Periodic Table of the Elements

1s
2s
3s

	1	2											3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18				
①	1 H																												2 He			
②	3 Li	4 Be																						5 B	6 C	7 N	8 O	9 F	10 Ne			
③	11 Na	12 Mg																						13 Al	14 Si	15 P	16 S	17 Cl	18 Ar			
④	19 K	20 Ca											21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr				
⑤	37 Rb	38 Sr											39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe				
⑥	55 Cs	56 Ba	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
⑦	87 Fr	88 Ra	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og

l=2
l=2
l=3 f

m_l = 2, 1, 0, -1, -2

l=4 g? 18 e⁻

The Aufbau Principle

1. Start at the lowest quantum level and fill up

Start at $n=1$

2. Pauli exclusion principle

can't have identical quantum numbers

He e_1 $n=1$ $l=0$ $m_l=0$ $m_s=+\frac{1}{2}$
 e_2 $n=1$ $l=0$ $m_l=0$ $m_s=-\frac{1}{2}$

$\uparrow\downarrow$

~~$\uparrow\uparrow$~~

3. Hund's Rule of Multiplicity--Multiplicity is the number of unpaired e^- 's + 1

He $\uparrow\downarrow$ this is a singlet state 0 unpaired e^- 's + 1 = 1

H \uparrow this is a doublet state 1 unpaired e^- + 1 = 2

arrange e^- so that they have the highest possible multiplicity

4. Exchange Energy/Exchange Interaction

$\uparrow\uparrow$ vs $\uparrow\downarrow$
 says this is more stable

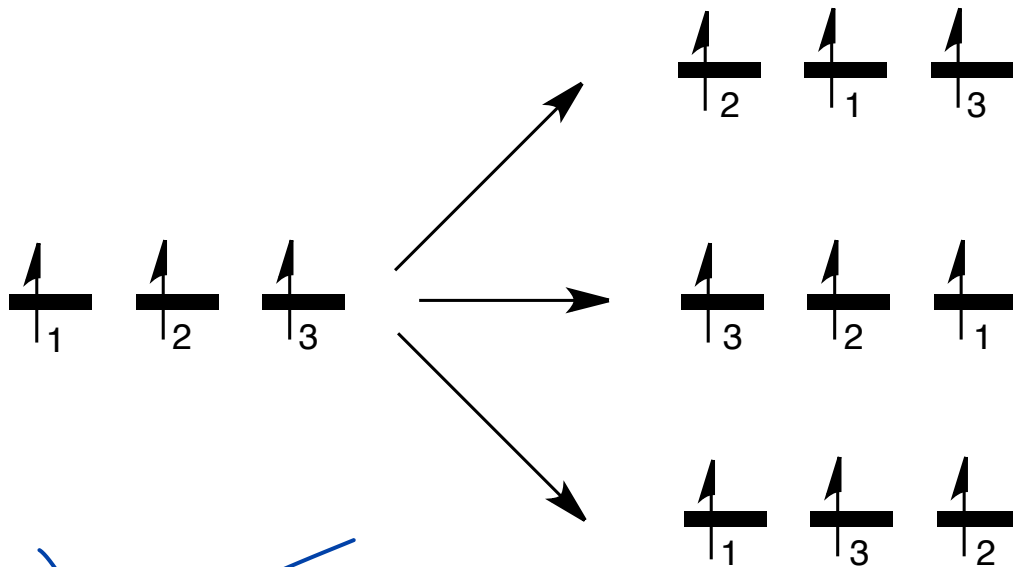
1 e^- in a set of degenerate orbitals... doesn't matter which orbital is occupied

\uparrow — —

$\uparrow\downarrow$ — — or $\uparrow\uparrow$ — —

A quantum mechanical effect that exists between identical particles

Particles aren't actually changing positions - it is more about what happens if they were to change positions. If there would be no change, then with respect to that exchange the the change is symmetric. Symmetrical exchange for electrons spin states means that there is spacial component of the wave function is antisymmetric. There is slightly more distance between particles that have antisymmetry spacial wave functions than those with symmetric spacial wave functions. Thus, lower E.



~~↑ ↓ ↑~~
 by convention e^- 's are placed spin up first

↑ ↑ ↓
 ↑ ↑
 not aligned
 exchange would be antisymmetric
 space wave function would be symmetric and the e^- 's would experience greater $e^- - e^-$ repulsion

1. start in lowest quantum levels
2. Pauli exclusion principle
 - no two electrons in an atom or molecule can have identical quantum numbers
3. Hund's Rule of Multiplicity
 - multiplicity is the number of unpaired e⁻'s + 1
 - the lowest energy state for electrons in degenerate orbitals is the one with the highest multiplicity
 - electrons only pair after all degenerate orbitals have been half filled
4. Exchange interaction
 - spin aligned electrons in degenerate orbitals are lower in energy than those that aren't spin aligned

Rationalizing electron configurations/Factors affecting the energy of the electron

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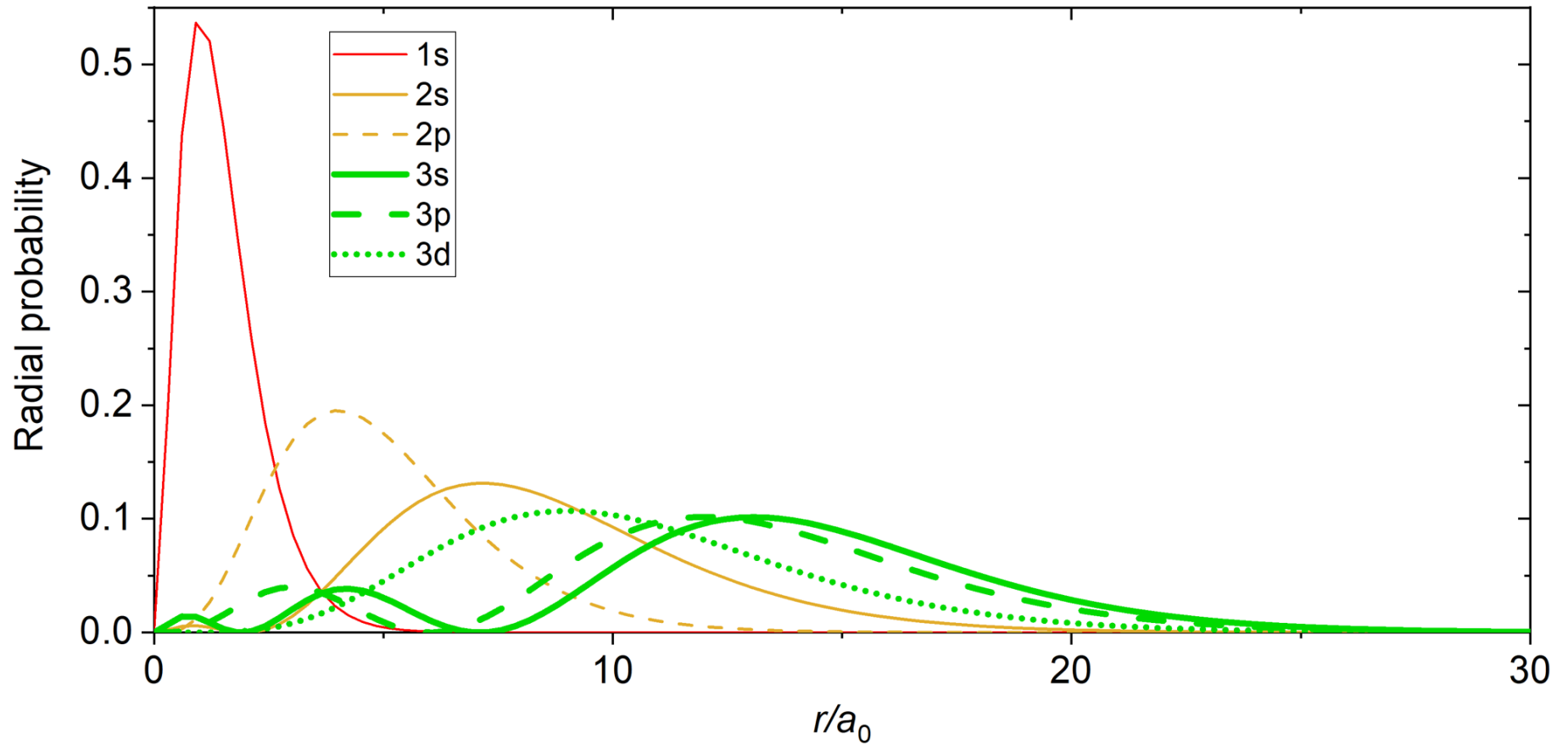
Penetration and effective nuclear charge

Π_c = coulomb repulsion

- bad
- number of paired electrons

Π_e = exchange energy

- good in the case of parallel electrons in degenerate orbitals in an atom
- number of exchanges that can be made and produce identical electron configurations

Penetration and effective nuclear charge

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Wave Functions

http://www.westfield.ma.edu/cmasi/advinorg/angular_distribution_functions/text_and_graphics_containe.htm

