(4) **Today**

2.2.2 Quantum Numbers and Atomic Wave Functions

2.2.3 The Aufbau Principle

2.2.4 Shielding

Next Class (5)

2.3 Periodic Properties

(6) **Second Class from Today**

2.3 Periodic Properties

3.1 Lewis Structures

3.2 VSEPR

Third Class from Today (7)

3.2 VSEPR

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, 2, 3, 4

l is the Angular momentum quantum number

allowed values are the from n - 1 to 0 in whole number increments

$n=1$ $l = 1-1 = 0$ s orbital

$n=2$ & $l=0$ s orbital $l = 2-1 = 1$ p orbitals 3 2p orbitals

m_l is the magnetic quantum number

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

$l = 0$ $M_l = 0$

$l = 1$ $M_l = -1, 0, 1$

in $n=3$ ... $l=2$ now exists

3d 5 3d orbital

$M_l = -2, -1, 0, 1, 2$

m_s is the spin quantum number

allowed values are - ½ or +½

The Aufbau Principle

1. Start at the lowest quantum level and fill up

start at n=1 and fill up from there ... no gaps

2. Pauli exclusion principle

e⁻'s need to be spin paired when placed in the same orbital

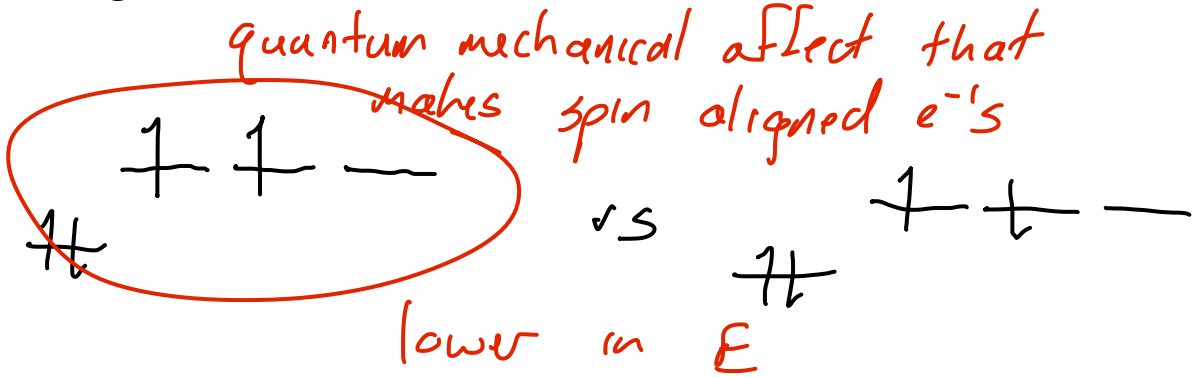
$m_s = \frac{1}{2}$ $m_s = -\frac{1}{2}$ ↑↓

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

in degenerate orbitals (orbitals with the same energy)

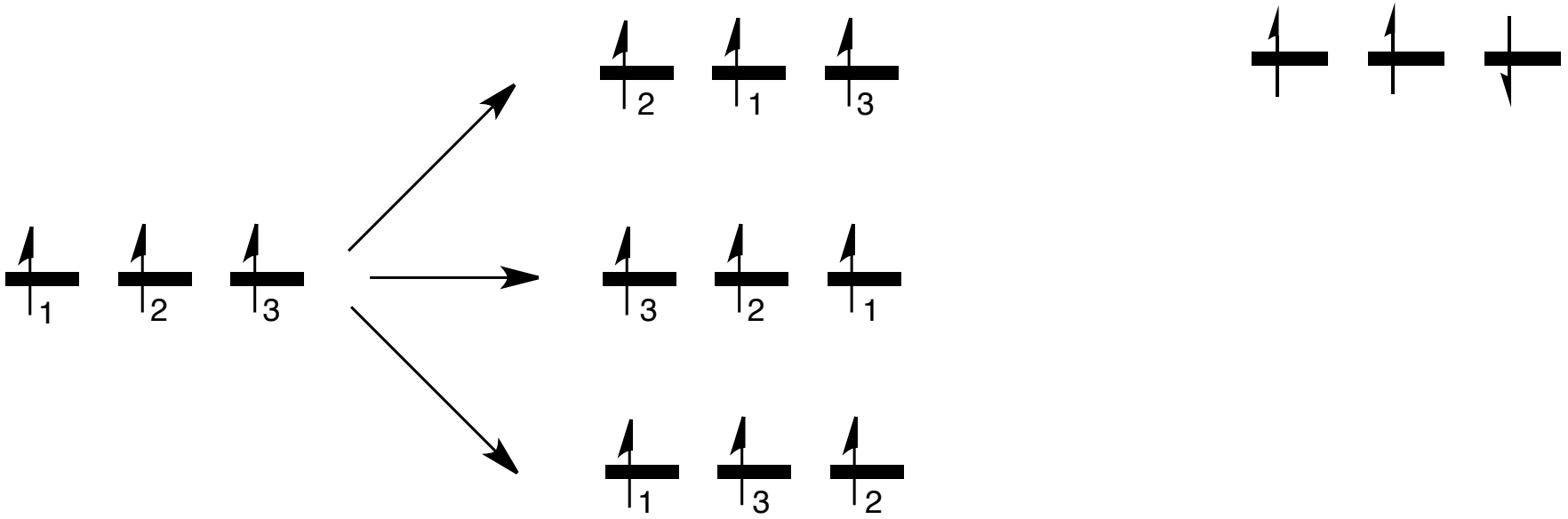
e⁻'s don't pair until absolutely necessary

4. Exchange Energy/Exchange Interaction



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.



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

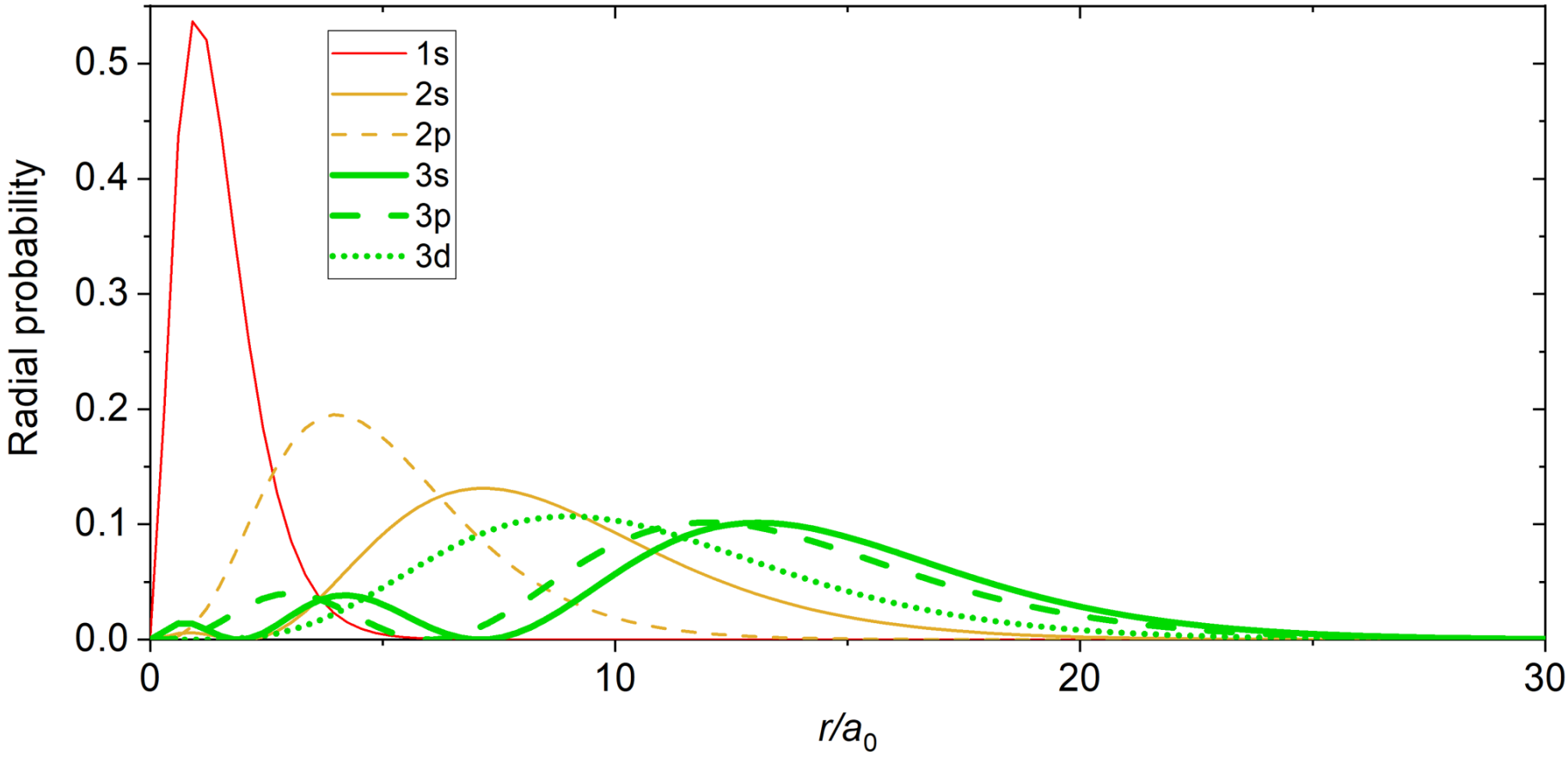
Rationalizing electron configurations/Factors affecting the energy of the electron

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

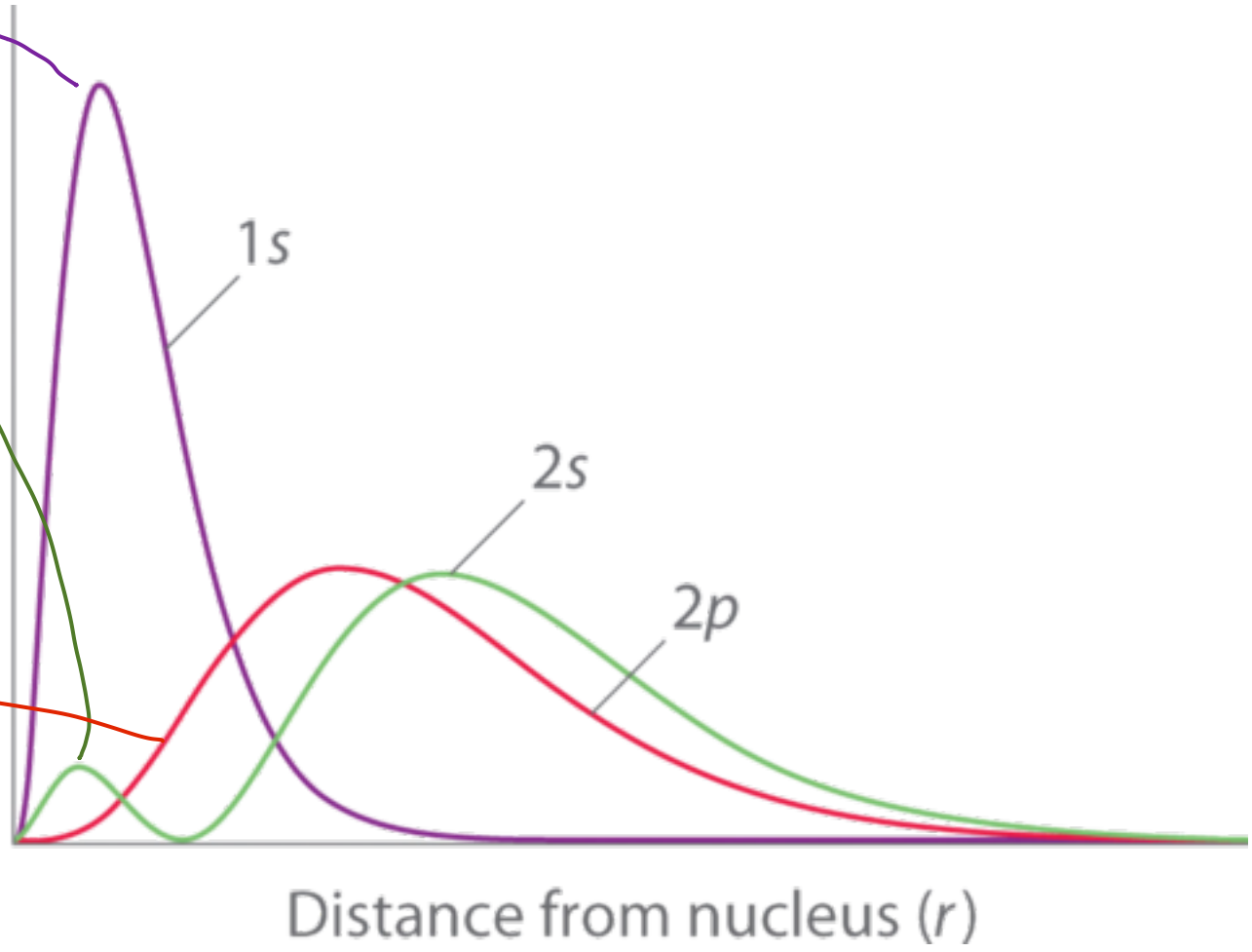


Penetration and effective nuclear charge

is e's spend a lot of time near the nucleus... low in E

2s orbitals penetrate closer to the nucleus an being super close makes 2s e⁻'s lower in E than p e⁻'s

don't penetrade as close to the nucleus



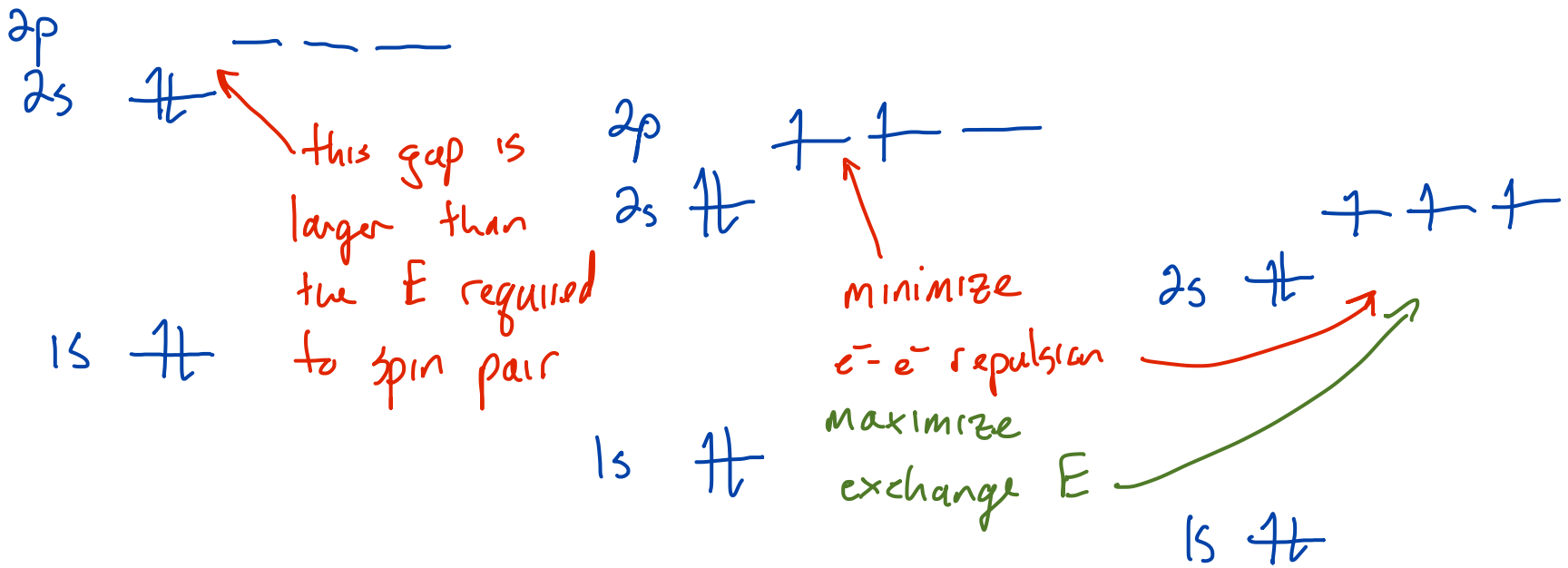
https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Inorganic_Chemistry_(LibreTexts)/02%3A_Atomic_Structure/2.02%3A_The_Schrodinger_equation_particle_in_a_box_and_atomic_wavefunctions/2.2.04%3A_Shielding accessed 9/15/2023

Orbitals are represented as lines. Lower E orbitals are drawn at the bottom of the page

Periodic Table of the Elements

	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

Be $1s^2\ 2s^2$ C $1s^2\ 2s^2\ 2p^2$ N $1s^2\ 2s^2\ 2p^3$



Periodic Table of the Elements

	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

Cr [Ar] $4s^2 3d^4$

Mn [Ar] $4s^2 3d^5$

4p
3d
4s
[Ar]

$4s^1 3d^5$

e⁻-e⁻ repulsion reduced
exchange E maximized

4p
3d
4s
[Ar]

maximize exchange E
which is good

3d
4s

e⁻-e⁻ repulsion

wrong