Now to build Helium...

The Pauli Exclusion Principle requires...

totally antisymmetric wavefunctions.

$$\Psi_T \text{ (both electrons)} = \Psi_S \Sigma_A \qquad \text{singlet} \quad 1 \text{ state}$$

$$\text{or} \qquad = \Psi_A \Sigma_S \qquad \text{triplet} \quad 3 \text{ states}$$

Energy...

$$E_T = -\frac{\mu z^2 e^4}{(4\pi\epsilon_0)^2 2\hbar^2 n_1^2} - \frac{\mu z^2 e^4}{(4\pi\epsilon_0)^2 2\hbar^2 n_2^2}$$

$z = 2$.

$$E_T = -4\frac{(13.6\,eV)}{n_1^2} - 4\frac{(13.6\,eV)}{n_2^2}$$

Ground state:

$$n_1 = n_2 = 1$$

$$E_T(g.s.) = -(4+4)(13.6) = -109\,eV$$

1st Excited State: $n_1 = 1$ or 2 and $n_2 = 2$ or 1

$$E_T(1st) = -(4+1)(13.6) = -68\,eV$$

The coulomb force between the 2e raises these values...

But... it's more complicated than this.

The G.S. He calculation assumed that hydrogen assumptions could be used for each electron...

the OTHER electron... what does it "see"?

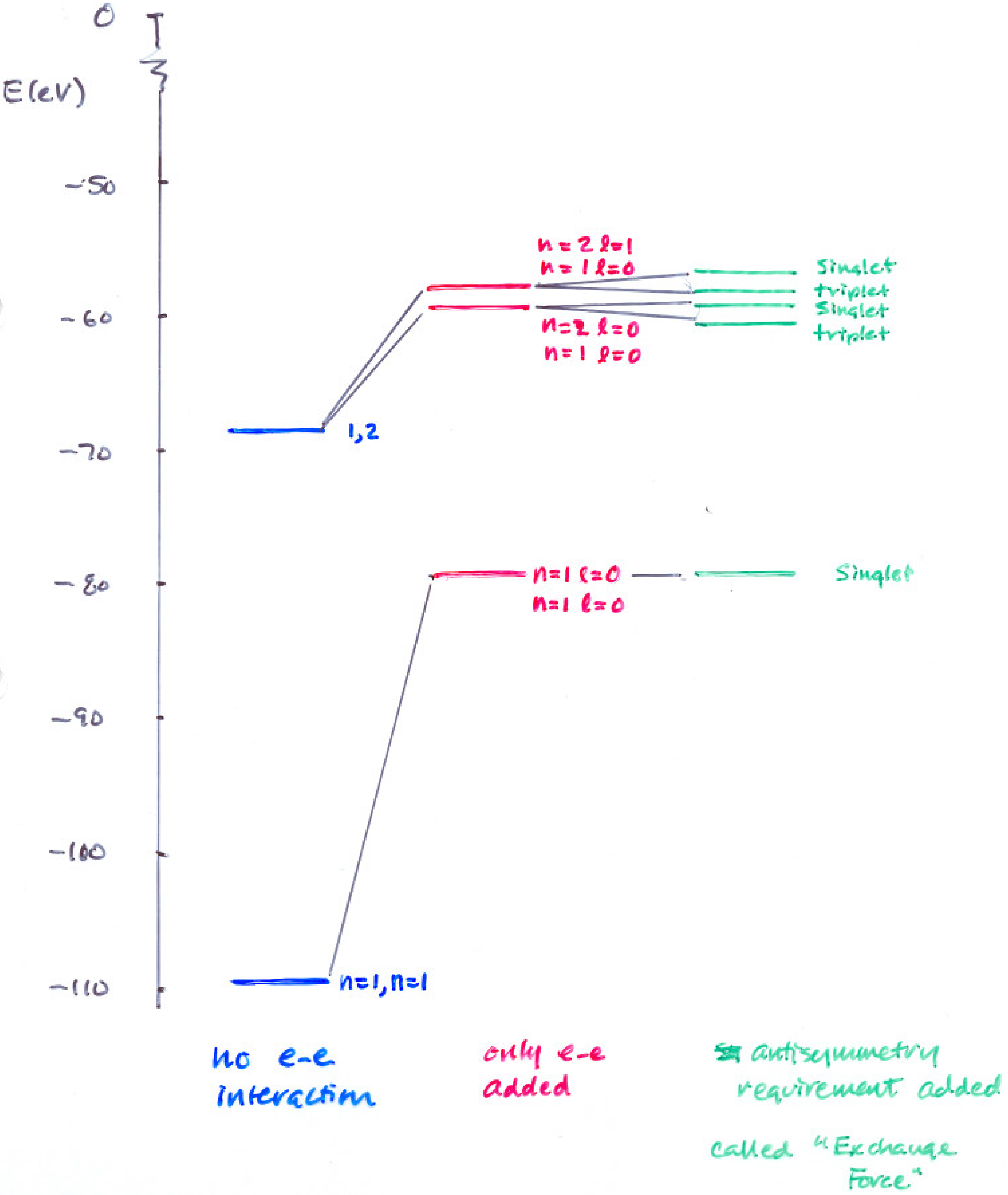
Not $Z = 2$ ... because its partner electron screens some of the positive nuclear charge.

An "effective" Z ... "Z^*" can be calculated & measured ... $Z^* = 1.7$ not 2 seen by either electron... so

$$E_T(g.s.) = -(1.7^2 + 1.7^2)(13.6) = -79 \text{ eV}$$

Now... remove an electron... ionize. What's left is a hydrogen-like atom $E_T(\text{ionized}) = -4(13.6) = 54.4 \text{ eV}$

So... what is the ionization energy of that first electron? 79 eV − 54.4 eV = 24.6 eV



SO...

even Helium is complicated!

The rest of the Periodic Table is too... rules of thumb

1. Electrons tend to the lowest energy levels
2. Pauli Exclusion Principle at work

an aside...

this separation of

spin ½ particles	Fermions
spin 0 & 1 particles	Bosons

we don't understand.

A theory called "supersymmetry" is of prime importance at the Large Hadron Collider in Genevé, Switzerland → merges the notions of half and whole integer-spin particles.

The old-time xray notation still sticks around:

$n=$	1	2	3	4
	K	L	M	N

Energy levels depends primarily on <u>n</u>.

speak of them as "shells"

K shell, L shell ... etc.

Further designation .. $n\ell$

speak of them as "subshells"

1s, 2p ... etc. subshells.

So.

electron state: (n, ℓ, m_ℓ, m_s)

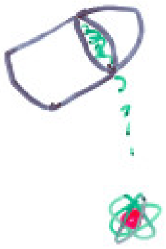
n → shell

ℓ → subshell

For no magnetic field → energy doesn't depend on m_ℓ or m_s

(ignoring any internal magnetic effects)

We speak of "filling the shells" like..



not really the case of course..

But, can account for energy levels and subshell occupation thinking this way..

SO... HOW MANY?

depends on the m_ℓ and m_s

depends on the ℓ. $(2\ell+1) = \#$

depends on the n. $n = \#$

m_ℓ

$\ell = 0$	"s"	$(2 \cdot 0 + 1) = 1$	value of m_ℓ	0
$\ell = 1$	"p"	$(2 \cdot 1 + 1) = 3$	values of m_ℓ	-1, 0, +1
$\ell = 2$	"d"	$(2 \cdot 2 + 1) = 5$	values of m_ℓ	-2, -1, 0, 1, 2

m_s

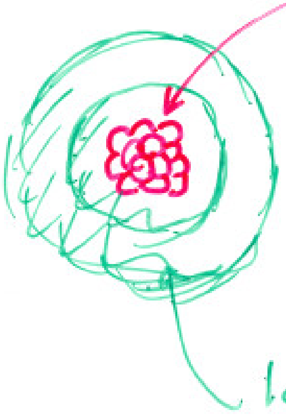
for each m_ℓ, $m_s = \pm 1/2$

n	ℓ	subshell	2ℓ+1	m_ℓ	max m_s		max states
1	0	1s	1	0	½ & -½	↑↓	2
2	0	2s	1	0	½ & -½	↑↓	2
2	1	2p	3	-1		↑↓	6
				0		↑↓	
				+1		↑↓	
3	0	3s	1	0		↑↓	2
3	1	3p	3	-1		↑↓	6
				0		↑↓	
				+1		↑↓	
3	2	3d	5	-2		↑↓	10
				-1		↑↓	
				0		↑↓	
				+1		↑↓	
				+2		↑↓	

⋮

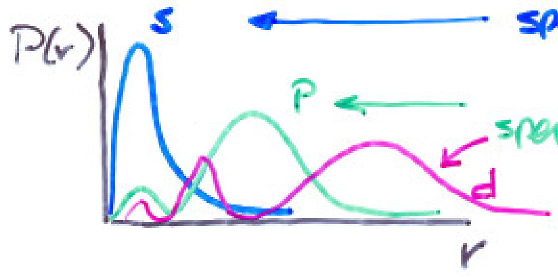
SHIELDING...

outer electrons don't "see" the entire nuclear charge...



- outer electrons see something less than +Ze
- and electrons "feel" each other!

ALSO... remember the radial probability distributions.

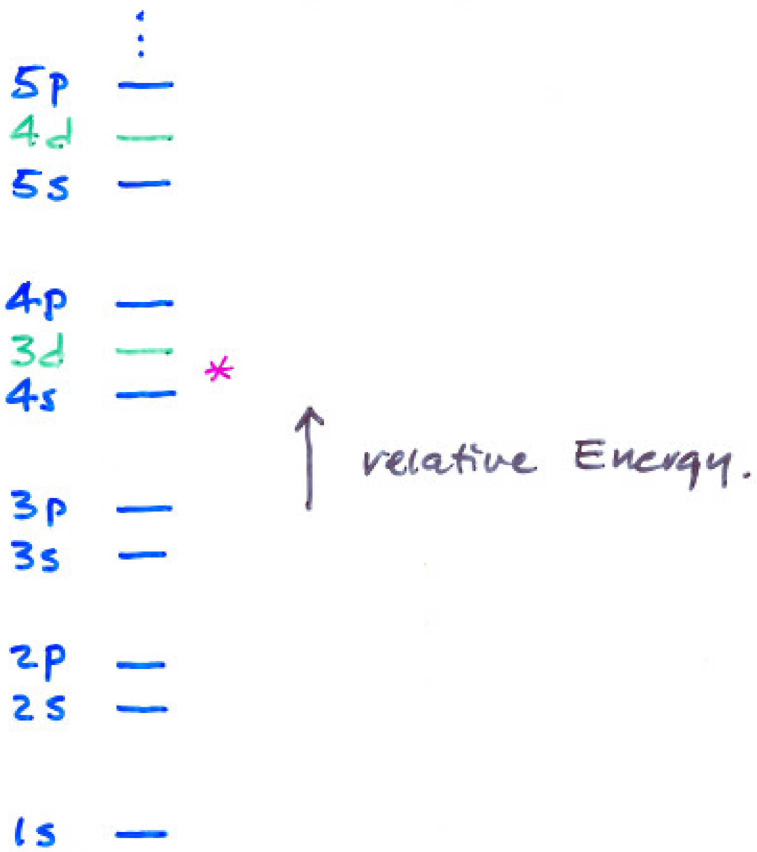


SO outer shell s electrons can be more tightly bound than inner shell d, or f...

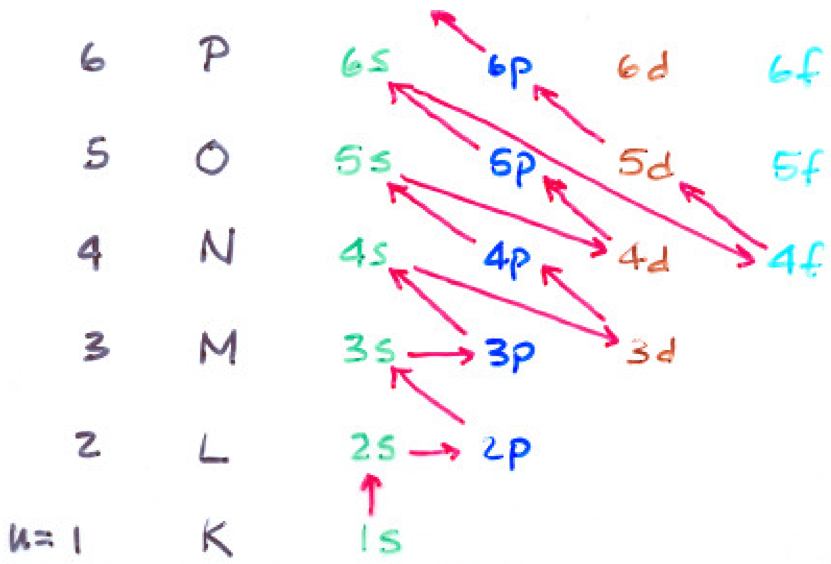
changing the ordering of which shell's "fill" when.

Actually goes like this...

presumes all inner shells are full... where will the next electron "go" (or better.. "be found")



or:



must come from tough calculations...

explains P.T.

H	(↑,) $1s^1$			
He	(↑,↓) $1s^2$			full
Li	(↑,↓) $1s^2$	(↑,) $2s^1$		
Be	(↑,↓) $1s^2$	(↑,↓) $2s^2$		
B	(↑,↓) $1s^2$	(↑,↓) $2s^2$	(↑,) (,) (,) $2p^1$	
C	(↑,↓) $1s^2$	(↑,↓) $2s^2$	(↑,) (↑,) (,) $2p^2$	
N	(↑,↓) $1s^2$	(↑,↓) $2s^2$	(↑,) (↑,) (↑,) $2p^3$	

etc.

⋮

Ne	(↑,↓) $1s^1$	(↑,↓) $2s^2$	(↑,↓) (↑,↓) (↑,↓) $2p^6$	full

Diversion to... CHEMISTRY

names: $_{Z}X$

atomic number (Z) = # protons = # electrons

X: chemical symbol

eg carbon: $_{6}C$

all about the outer electrons...

closed shells — Inert or Noble Gases

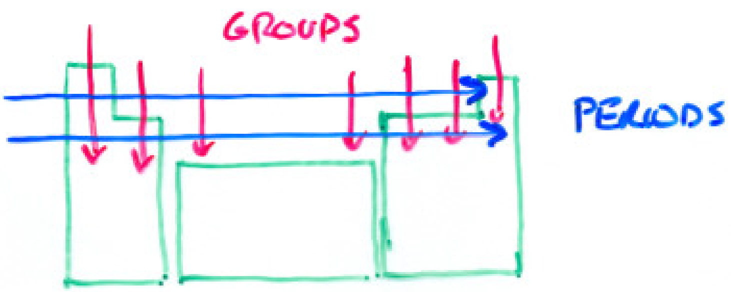
$_{2}He$ $1s^2$; $_{10}Ne$ $1s^2 2s^2 2p^6$; $_{18}Ar$ $1s^2 2s^2 2p^6 3s^2 3p^6$

single electron outside closed shells — Alkalis

$_{3}Li$ $2s^1$; $_{11}Na$ $1s^2 2s^2 2p^6 3s^1$

one electron short of closed shells — Halogens

$_{9}F$ $2s^2 2p^5$; $_{17}Cl$ $3s^2 3p^5$



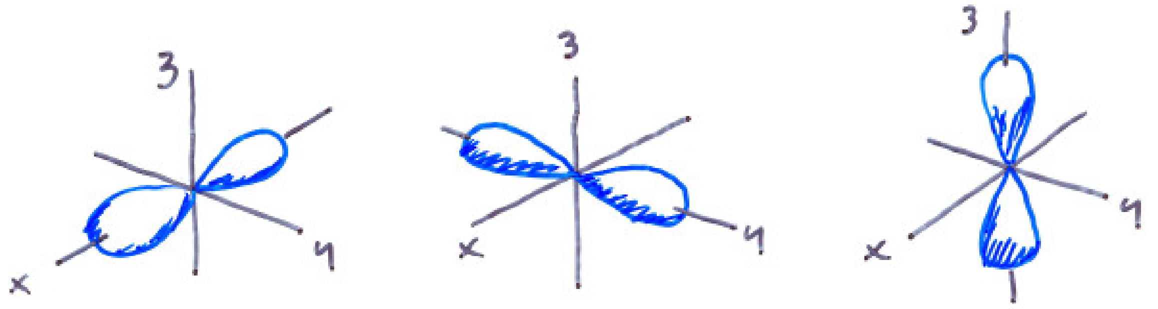
Carbon is interesting

6 C $1s^2 2s^2 2p^2$

where do those guys go?

These involve the spherical harmonics Y_{11}, Y_{10}, Y_{1-1}

In probability distributions they have lobes..



the 1st 2p electron can go into one lobe - "arm"

the 2nd 2p electron can go into an orthogonal one.

→ they can literally get away from one another

minimizing the repulsive energy

raising the ionization energy.

BUT WAIT.. THERE'S MORE

$1s^2 2s^2 2p^2 \longrightarrow 1s^2 2s\, 2p^3$ energetically easy

strongly bonding to other stuff

LIFE AS WE KNOW IT

s shells, 2

Closed shells	1 (Alkalis) +1	2 (Alkaline earths) +2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17 (Halogens) −1	18 (Rare gases)
	1 H $1s$																	2 He $1s^2$
$1s^2$	3 Li $2s^1$	4 Be $2s^2$											5 B $2s^2 2p^1$	6 C $2s^2 2p^2$	7 N $2s^2 2p^3$	8 O $2s^2 2p^4$	9 F $2s^2 2p^5$	10 Ne $2s^2 2p^6$
$2s^2 2p^6$	11 Na $3s^1$	12 Mg $3s^2$											13 Al $3s^2 3p^1$	14 Si $3s^2 3p^2$	15 P $3s^2 3p^3$	16 S $3s^2 3p^4$	17 Cl $3s^2 3p^5$	18 Ar $3s^2 3p^6$
$3s^2 3p^6$	19 K $4s^1$	20 Ca $4s^2$	21 Sc $3d^1 4s^2$	22 Ti $3d^2 4s^2$	23 V $3d^3 4s^2$	24 Cr $3d^5 4s^1$	25 Mn $3d^5 4s^2$	26 Fe $3d^6 4s^2$	27 Co $3d^7 4s^2$	28 Ni $3d^8 4s^2$	29 Cu $3d^{10} 4s^1$	30 Zn $3d^{10} 4s^2$	31 Ga $3d^{10} 4s^2 4p^1$	32 Ge $3d^{10} 4s^2 4p^2$	33 As $3d^{10} 4s^2 4p^3$	34 Se $3d^{10} 4s^2 4p^4$	35 Br $3d^{10} 4s^2 4p^5$	36 Kr $3d^{10} 4s^2 4p^6$
$3d^{10} 4s^2 4p^6$	37 Rb $5s^1$	38 Sr $5s^2$	39 Y $4d^1 5s^2$	40 Zr $4d^2 5s^2$	41 Nb $4d^4 5s^1$	42 Mo $4d^5 5s^1$	43 Tc $4d^6 5s^1$	44 Ru $4d^7 5s^1$	45 Rh $4d^8 5s^1$	46 Pd $4d^{10}$	47 Ag $4d^{10} 5s^1$	48 Cd $4d^{10} 5s^2$	49 In $4d^{10} 5s^2 5p^1$	50 Sn $4d^{10} 5s^2 5p^2$	51 Sb $4d^{10} 5s^2 5p^3$	52 Te $4d^{10} 5s^2 5p^4$	53 I $4d^{10} 5s^2 5p^5$	54 Xe $4d^{10} 5s^2 5p^6$
$4d^{10} 5s^2 5p^6$	55 Cs $6s^1$	56 Ba $6s^2$	57 La $5d^1 6s^2$	72 Hf $4f^{14} 5d^2 6s^2$	73 Ta $4f^{14} 5d^3 6s^2$	74 W $4f^{14} 5d^4 6s^2$	75 Re $4f^{14} 5d^5 6s^2$	76 Os $4f^{14} 5d^6 6s^2$	77 Ir $4f^{14} 5d^9$	78 Pt $4f^{14} 5d^9 6s^1$	79 Au $4f^{14} 5d^{10} 6s^1$	80 Hg $4f^{14} 5d^{10} 6s^2$	81 Tl $4f^{14} 5d^{10} 6s^2 6p^1$	82 Pb $4f^{14} 5d^{10} 6s^2 6p^2$	83 Bi $4f^{14} 5d^{10} 6s^2 6p^3$	84 Po $4f^{14} 5d^{10} 6s^2 6p^4$	85 At $4f^{14} 5d^{10} 6s^2 6p^5$	86 Rn $4f^{14} 5d^{10} 6s^2 6p^6$
$4f^{14} 5d^{10} 6s^2 6p^6$	87 Fr $7s^1$	88 Ra $7s^2$	89 Ac $6d^1 7s^2$	104 Rf $5f^{14} 6d^2 7s^2$	105 Db $5f^{14} 6d^3 7s^2$	106 Sg $5f^{14} 6d^4 7s^2$	107 Bh $5f^{14} 6d^5 7s^2$	108 Hs $5f^{14} 6d^6 7s^2$	109 Mt $5f^{14} 6d^7 7s^2$	110 Ds $5f^{14} 6d^9 7s^1$	111 Rg $5f^{14} 6d^{10} 7s^1$	112 $5f^{14} 6d^{10} 7s^2$						

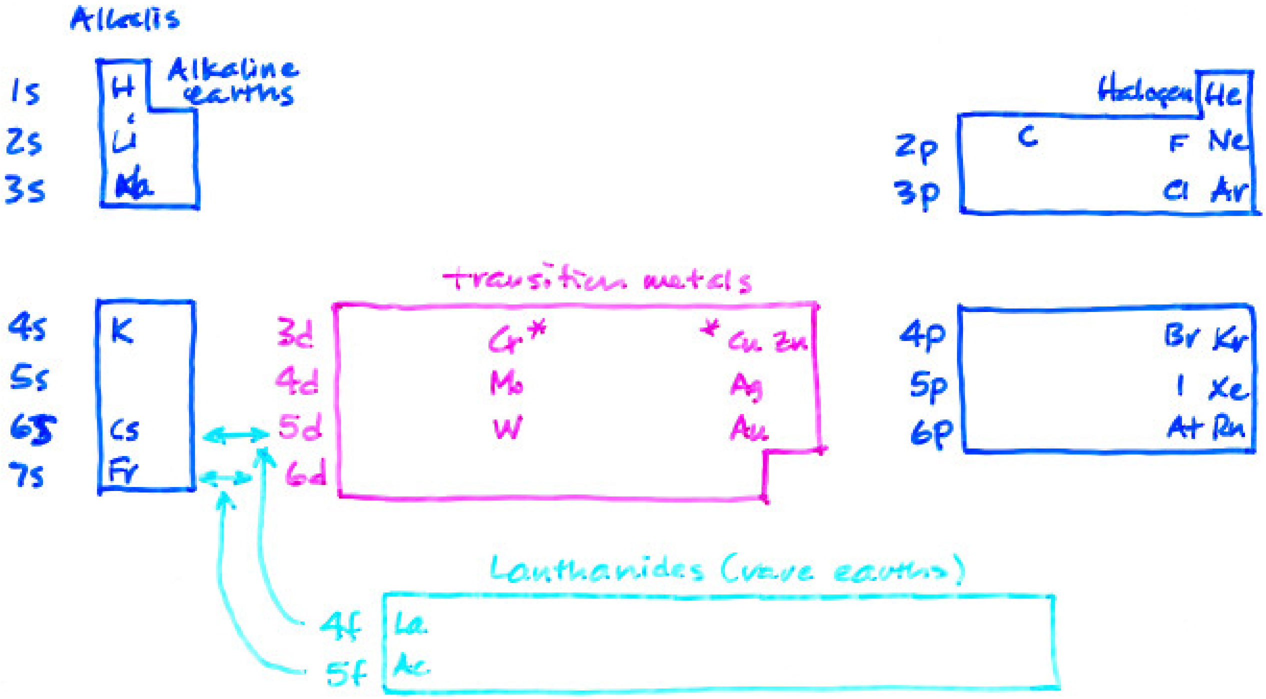
Groups 3–12: Transition elements — nd (n+1)s shells, 10

Groups 13–18: p shells, 6

Lanthanides	58 Ce $4f^2 6s^2$	59 Pr $4f^3 6s^2$	60 Nd $4f^4 6s^2$	61 Pm $4f^5 6s^2$	62 Sm $4f^6 6s^2$	63 Eu $4f^7 6s^2$	64 Gd $4f^7 6s^2 5d^1$	65 Tb $4f^9 6s^2$	66 Dy $4f^{10} 6s^2$	67 Ho $4f^{11} 6s^2$	68 Er $4f^{12} 6s^2$	69 Tm $4f^{13} 6s^2$	70 Yb $4f^{14} 6s^2$	71 Lu $4f^{14} 5d^1 6s^2$
Actinides	90 Th $6d^2 7s^2$	91 Pa $5f^2 6d^1 7s^2$	92 U $5f^3 6d^1 7s^2$	93 Np $5f^4 6d^1 7s^2$	94 Pu $5f^6 7s^2$	95 Am $5f^7 7s^2$	96 Cm $5f^7 6d^1 7s^2$	97 Bk $5f^8 6d^1 7s^2$	98 Cf $5f^{10} 7s^2$	99 Es $5f^{11} 7s^2$	100 Fm $5f^{12} 7s^2$	101 Md $5f^{13} 7s^2$	102 No $5f^{14} 7s^2$	103 Lr $5f^{14} 6d^1 7s^2$

"rare earths"

f shells, 14



Through n=3 .. about what you would expect

1s (H) through $\underbrace{1s^2 2s^2 2p^6}_{Ne} 3s^2 3p^6$

$= [Ne] 3s^2 3p^6$

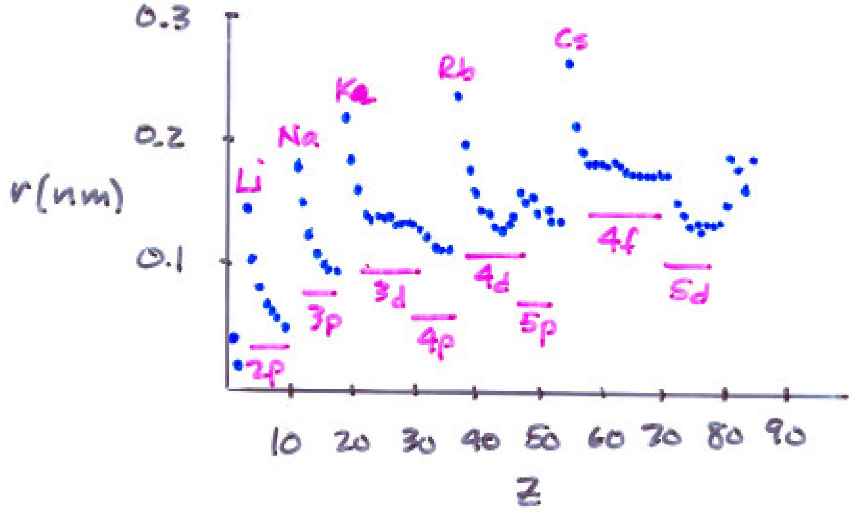
The 4th row gets strange

19	K:	$[Ar] 4s^1$	25	Mn	$[Ar] 3d^5 4s^2$
20	Ca ~~Sc~~:	$[Ar] 4s^2$	26	Fe	$[Ar] 3d^6 4s^2$
21	Sc ~~Cr~~:	[Ar] ~~3s~~ $3d^1 4s^2$	27	Co	$[Ar] 3d^7 4s^2$
22	Ti :	$[Ar] 3d^2 4s^2$	28	Ni	$[Ar] 3d^8 4s^2$
23	V:	$[Ar] 3d^3 4s^2$	29	Cu	$[Ar] 3d^{10} 4s^1$ *
24	Cr:	$[Ar] 3d^5 4s$ *	30	Zn	$[Ar] 3d^{10} 4s^2$

Filled subshells → very stable   He is king

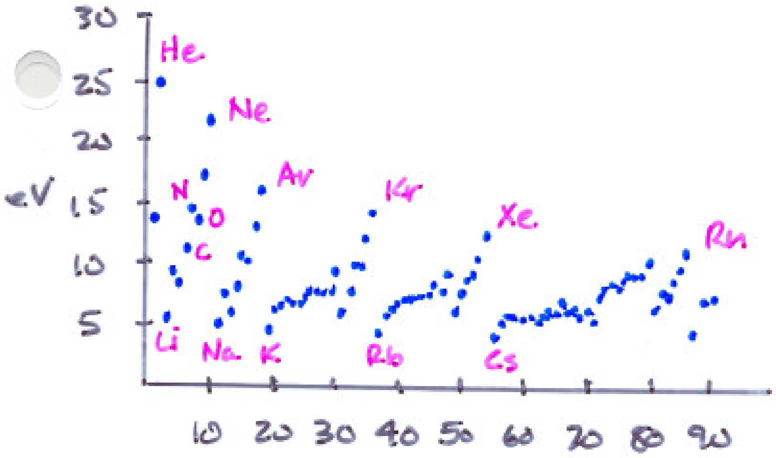
no chemistry

SIZE

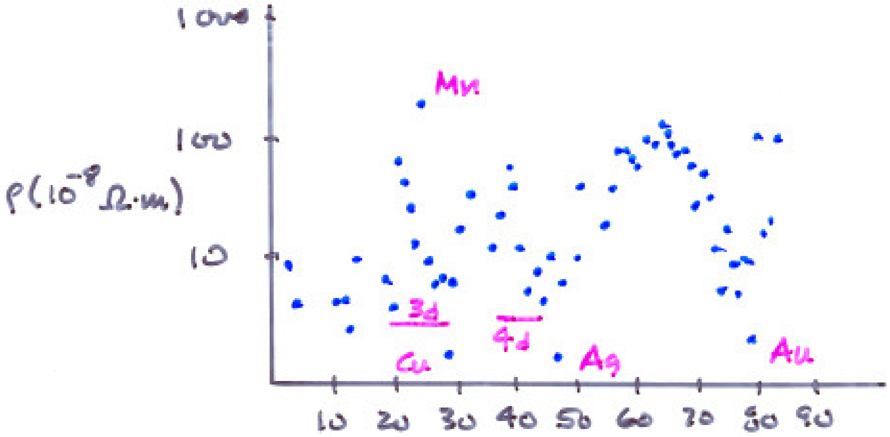


s shell electrons ... largest radii

IONIZATION ENERGY



RESISTIVITY

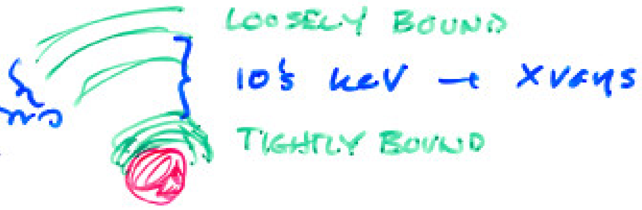


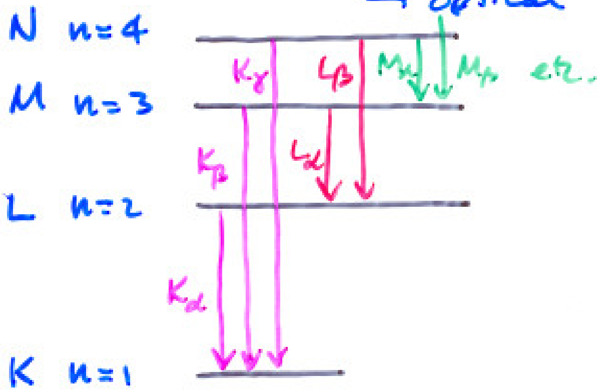
$$R = \rho \frac{L}{A}$$

* EXCITED * STATES

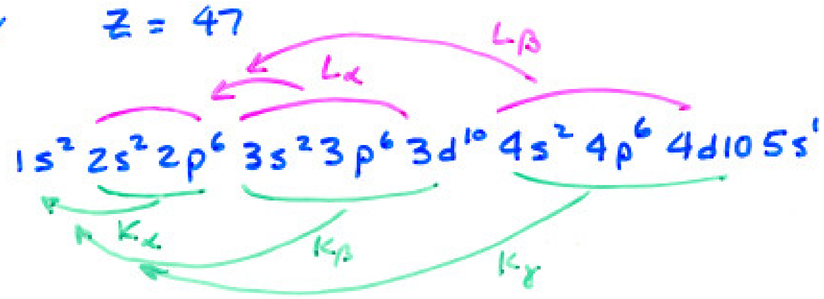
→ spectra

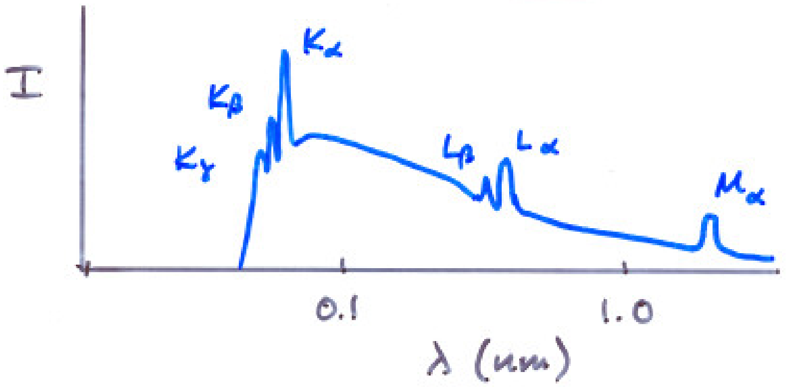
transitions
~ few eV
→ optical





silver Z = 47





Remember... takes 10's of kVolts to run xray machine

→ hard to kick ~~q~~ out an s electron