Quantum mechanics treats the electrons as waves and models THAT behavior!

- To describe the electrons, we use WAVEFUNCTIONs - which are mathematical descriptions of the behavior or electrons.
- The wavefunction describes the probability of finding an electron in a given space
- For larger objects, the wave behavior isn't very important .... and quantum mechanics becomes traditional Newtonian physics.

When we talk about describing electrons ... we will talk about the PARAMETERS that go into this WAVEFUNCTION ... without doing the actual math.

- There are FOUR of these parameters. (the Bohr model had only one!)
- The parameters are called "quantum numbers"

① Principal quantum number

② Angular momentum quantum number

③ Magnetic quantum number

④ Spin quantum number

- Giving the four parameters will uniquely identify an electron around an atom. No two electrons in the same atom can share all four. These parameters are called QUANTUM NUMBERS.

① PRINCIPAL QUANTUM NUMBER (n):

- "energy level", "shell"
- Represents two things:
  - * The distance of the electron from the nucleus.
  - * Energy. "n" is one factor that contributes to the energy of the electron.

$n = 1, 2, 3, 4, \ldots$ (integers)

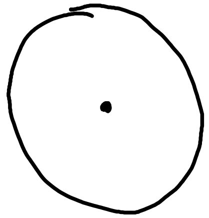
② ANGULAR MOMENTUM QUANTUM NUMBER: ℓ

- "subshell"
- Represents the SHAPE of the region of space where the electron is found.
  - (Bohr assumed CIRCULAR orbits for electrons ... but there are more possibilities.)

-"l" also contributes ENERGY. Higher values for "l" mean the electron has higher energy.

$\ell = 0$ to $n-1$, integers

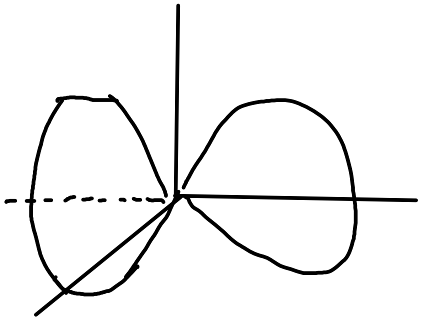
$n=1$; $\ell = 0$



"l" = 0 ; spherical subshell

Also called an "s" subshell.

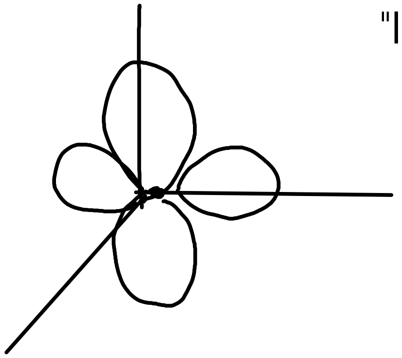
$n=2$; $\ell = 0, 1$



"l"=1 ; dumbbell shaped

Also called a "p" subshell

$n=3$, $\ell = 0, 1, 2$



"l"=2; flower-shaped

Also called a "d" subshell

Higher values for "l" translate to higher energies for the electron!

For convenience, and partially for historical reasons, we use letters to designate the different subshells.

$\ell=0$ "s"

$\ell=1$ "p"

$\ell=2$ "d"

$\ell=3$ "f"

$\ell=4$ "g"

↓ The rest follow the alphabet

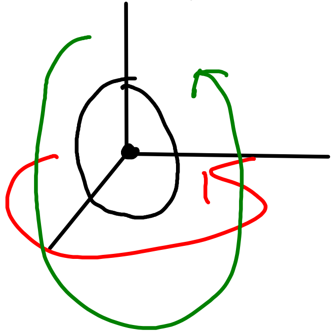
See page 305 in OpenStax for 3D pictures of the subshells

③ MAGNETIC QUANTUM NUMBER m_ℓ

- Represents the ORIENTATION of a subshell in 3D space.

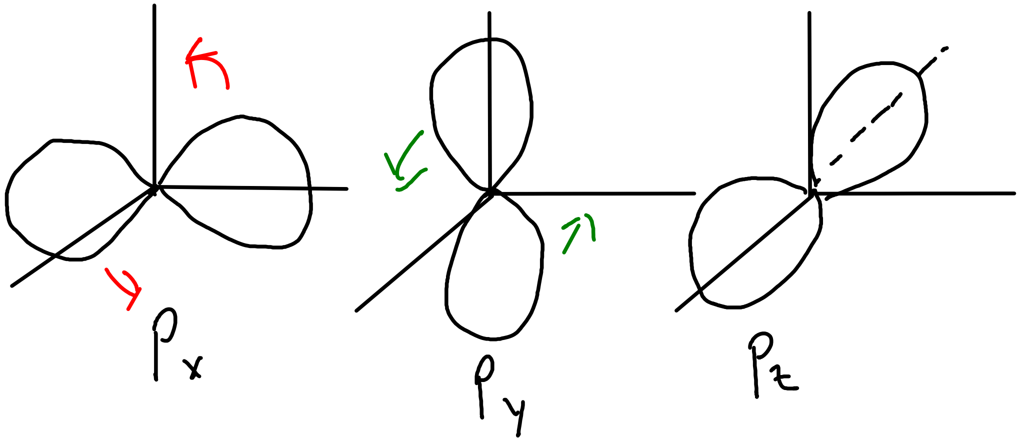
$m_\ell = -\ell$ to $+\ell$, integers

$\ell = 0$, $m_\ell = 0$
"s"



There is only one possible orientation for an "s" subshell!

$\ell = 1$; $m_\ell = -1, 0, 1$
"p"



There are THREE possible orientations for a "p" subshell!

$\ell = 2$, $m_\ell = -2, -1, 0, 1, 2$ (five orentations)
"d"

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in OpenStax

$\ell = 3$, $m_\ell = -3, -2, -1, 0, 1, 2, 3$ (seven orentations)
"f"

... all the arrangements of a single subshell have the same energy. The magnetic quantum number DOESN'T contribute to the energy of an electron.

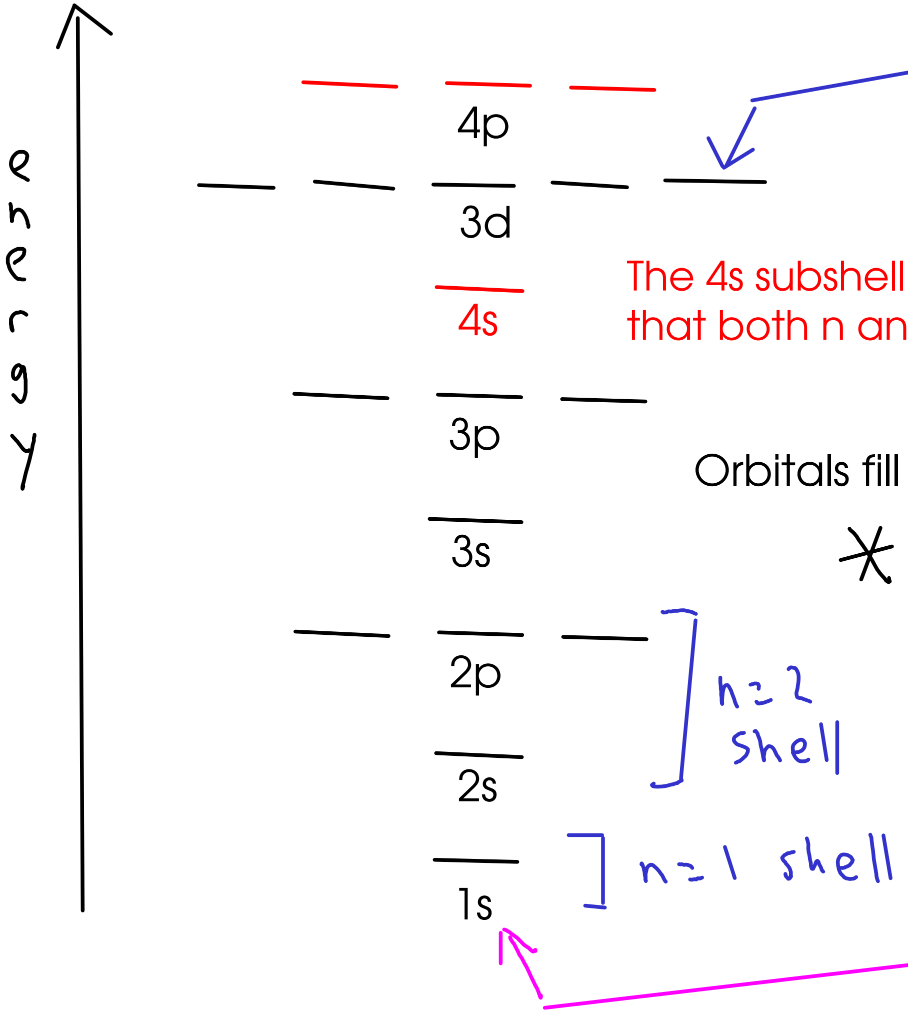
④ (MAGNETIC) SPIN QUANTUM NUMBER: m_s

$m_s = -1/2$ or $+1/2$ "spin down" or "spin up"

- An ORBITAL (region with fixed "n", "l" and "ml" values) can hold TWO electrons.

ORBITAL DIAGRAM

- A graphical representation of the quantum number "map" of electrons around an atom.



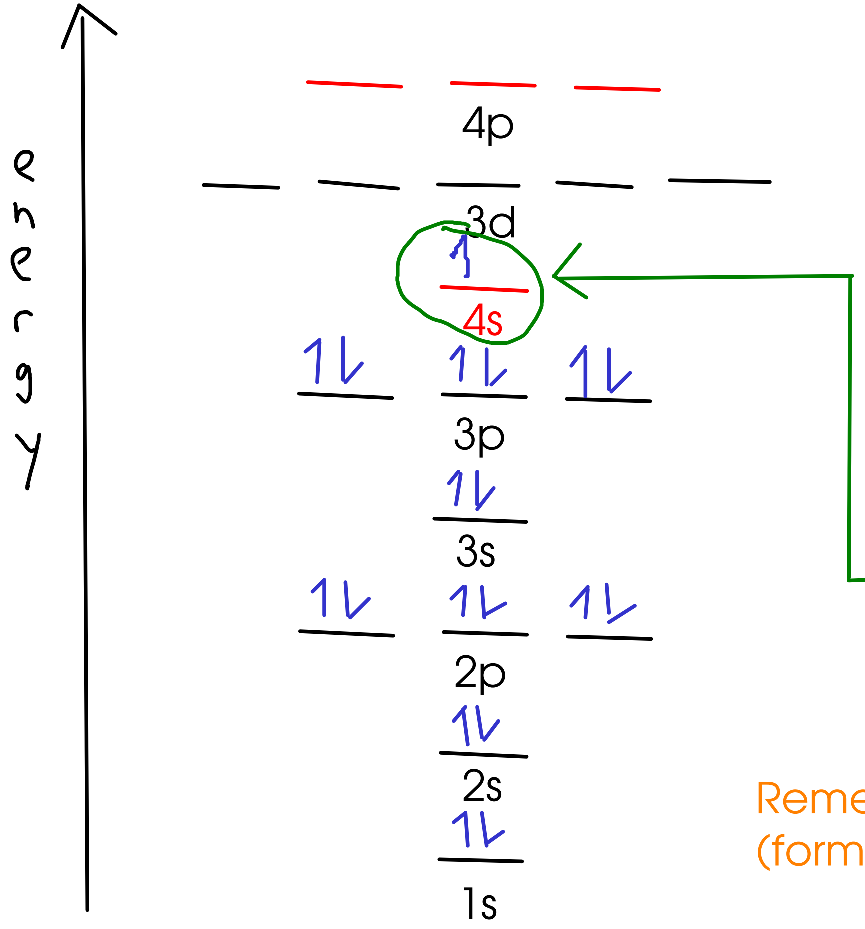
Each blank represents an ORBITAL, and can hold two electrons.

The 4s subshell is lower energy than the 3d subshells .... remember that both n and "l" contribute to energy!

Orbitals fill in order: The lower energy orbitals fill first.

* Where there's more than one orbital with the same energy, electrons don't pair up until each one has one electron in it!

1s: This means the first shell (n=1) and the "s" subshell ("l"=0)



How would an orbital diagram for the element POTASSIUM look?

K , Z = 19

Z – atomic number

Electrons in the outermost shell of an atom are called VALENCE electrons. THESE electrons are normally involved in chemical bonding.

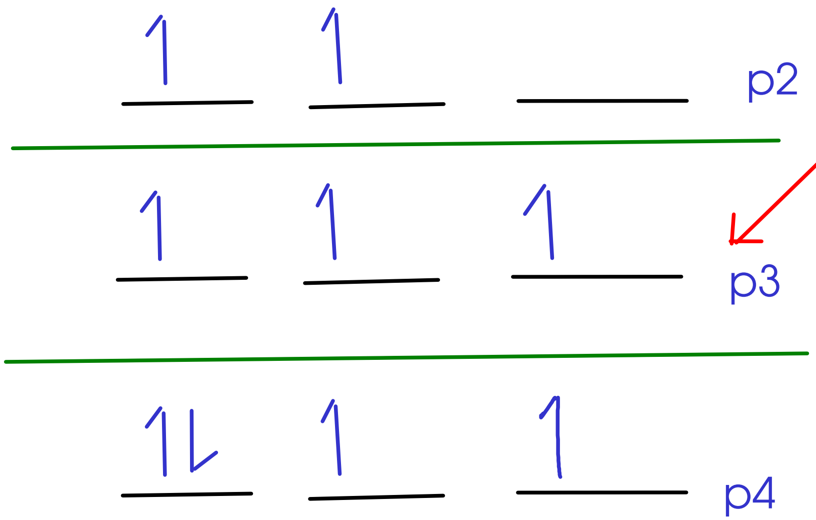
Remember: Potassium tends to lose a single electron (forming a cation) in chemical reactions. K^+

A note on chemical bonding and electron arrangement:

- Filled and half-filled subshells seem to be preferred by atoms.

HUND'S RULE

- When you have two or more orbitals with equivalent energy, electrons will go into each equivalent orbital BEFORE pairing. Pairing costs a bit of energy - less than going to a higher-energy orbital, but more than going to another equivalent orbital.



Electron configurations with filled subshells OR HALF-FILLED SUBSHELLS are more stable than other configurations.

(can explain some transition metal chemistry)

Electrons begin to pair only AFTER all equivalent "p" orbitals are full.

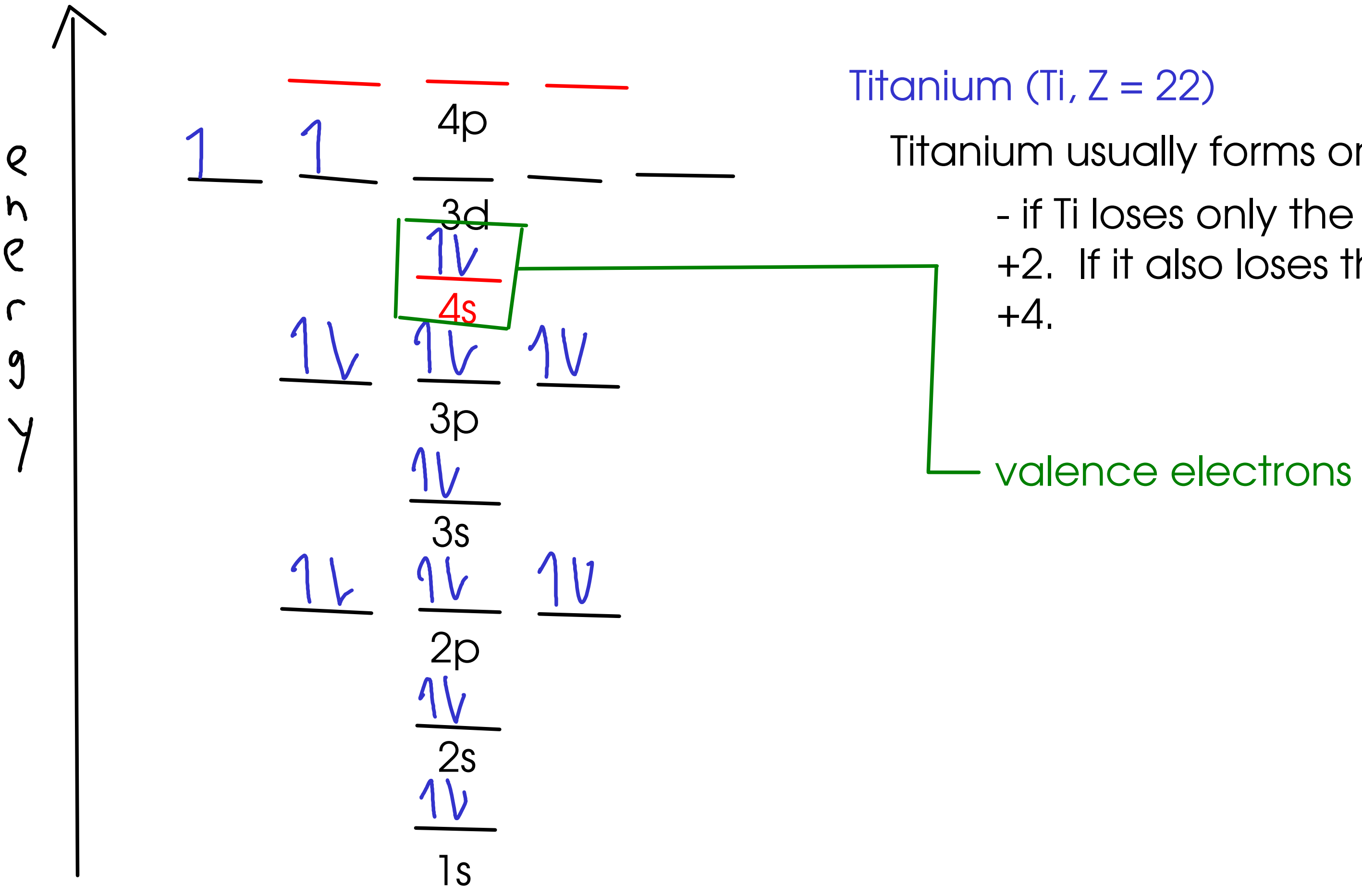
Experimental evidence for Hund's rule:

"Paramagnetism" - attraction of an atom to a magnetic field

* Spinning electrons are magnetic, but OPPOSITE spins cancel each other out.

* Atoms with unpaired electrons are paramagnetic, while atoms containing only paired electrons are not.

A little bit about transition metals...



Titanium (Ti, Z = 22)

Titanium usually forms one of two ions: +2 and +4

- if Ti loses only the valence electrons, forms +2. If it also loses the 3d electrons, forms +4.

- Most transition metals have TWO valence electrons (in an "s" subshell), and the other ions they form come from electron loss in "d" subshells.

ELECTRON CONFIGURATION (SHORT FORM)

- We can represent the electron configuration without drawing a diagram or writing down pages of quantum numbers every time. We write the "electron configuration".

# of electrons in the subshell

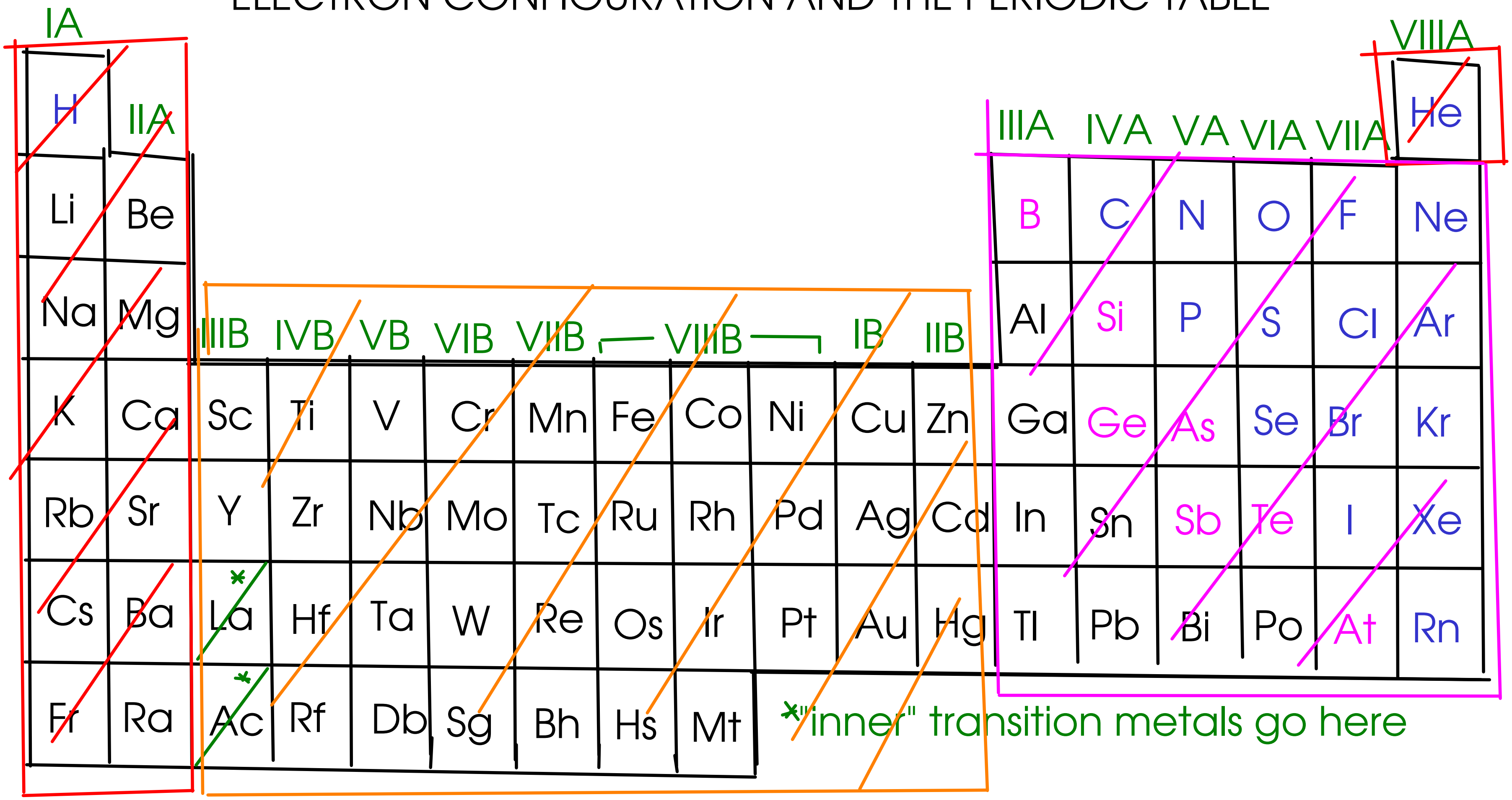
$$\text{Ti}: \underbrace{1}_{n}\underbrace{s}_{\ell}{}^{2}\,2s^{2}\,2p^{6}\,3s^{2}\,3p^{6}\,3d^{2}\,\underbrace{4s^{2}}_{\text{valence electrons}}$$

Valence electrons have the largest value for "n"!

$$\text{Ti}: \underbrace{[\text{Ar}]}\,3d^{2}\,\underbrace{4s^{2}}_{\text{valence electrons}}$$

"noble gas core". We're saying that titanium has the same electron configuration as argon does, with the addition of the electrons that follow. This is a useful shorthand, since the "core" electrons generally don't get involved in bonding.

ELECTRON CONFIGURATION AND THE PERIODIC TABLE



IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB			IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA
H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	*La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	*Ac	Rf	Db	Sg	Bh	Hs	Mt									

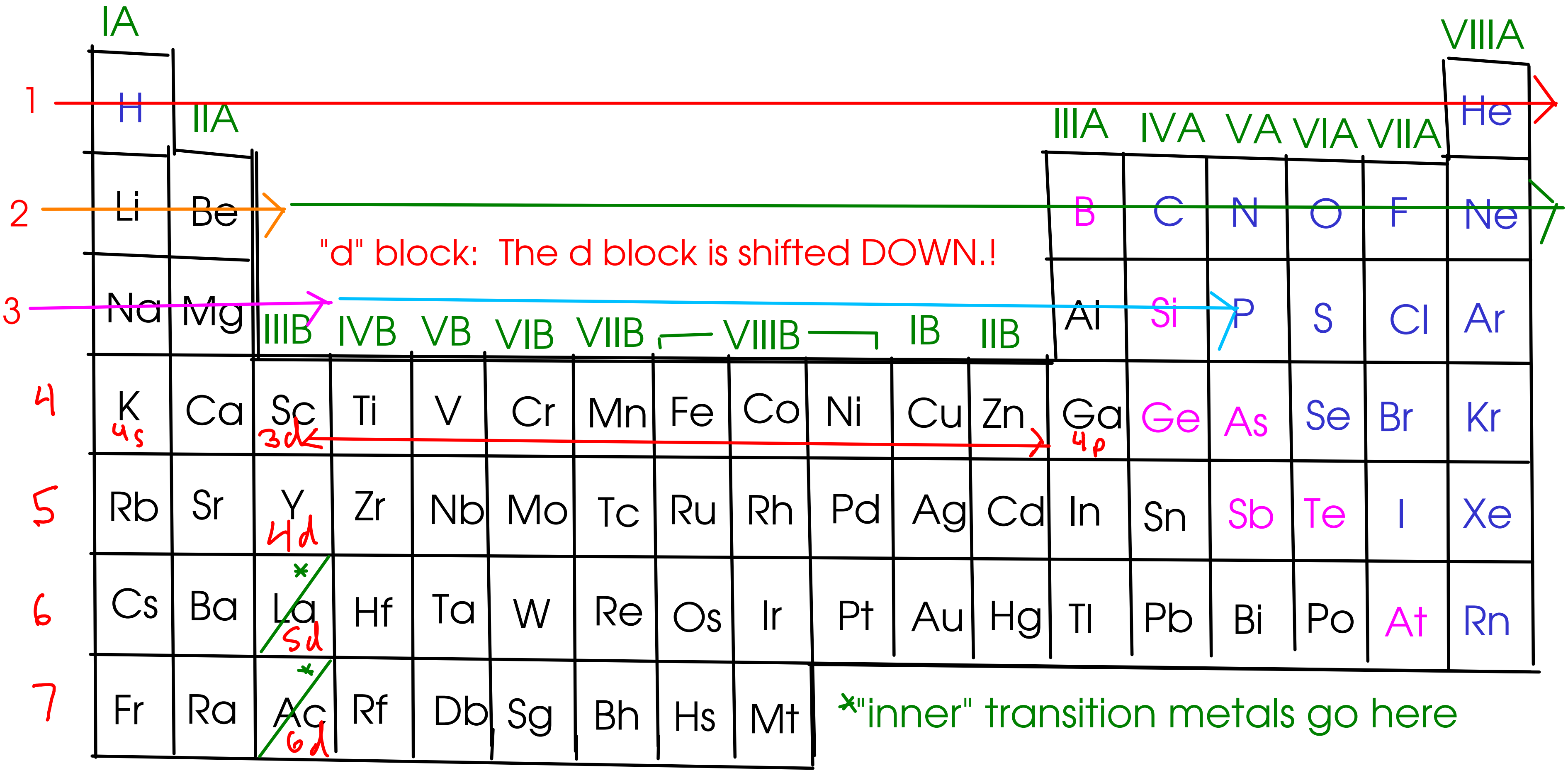
*"inner" transition metals go here

"s" block: last electron in these atoms is in an "s" orbital!

"p" block: last electron in these atoms is in a "p" orbital!

"d" block: last electron in these atoms is in a "d" orbital

- To write an electron configuration using the periodic table, start at hydrogen, and count up the electrons until you reach your element!



"d" block: The d block is shifted DOWN.!

	IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB	VIIIB	VIIIB	IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA
1	H																	He
2	Li	Be											B	C	N	O	F	Ne
3	Na	Mg											Al	Si	P	S	Cl	Ar
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	La*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	Ac*	Rf	Db	Sg	Bh	Hs	Mt									

*"inner" transition metals go here

Example: Phosphorus (P): $1s^2 2s^2 2p^6 3s^2 3p^3$

Noble gas core notation for P: $[Ne]\,3s^2 3p^3$