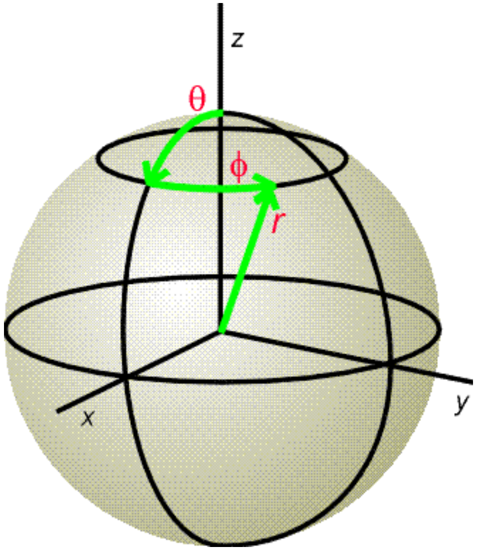
CHM2311
Introduction to Structure & Bonding

Part 1

Atomic Structure and Quantum Theory

Atomic Orbitals, Electron Density and Radial Probability



$\boxed{\psi}$ *atomic orbital (wave function)*

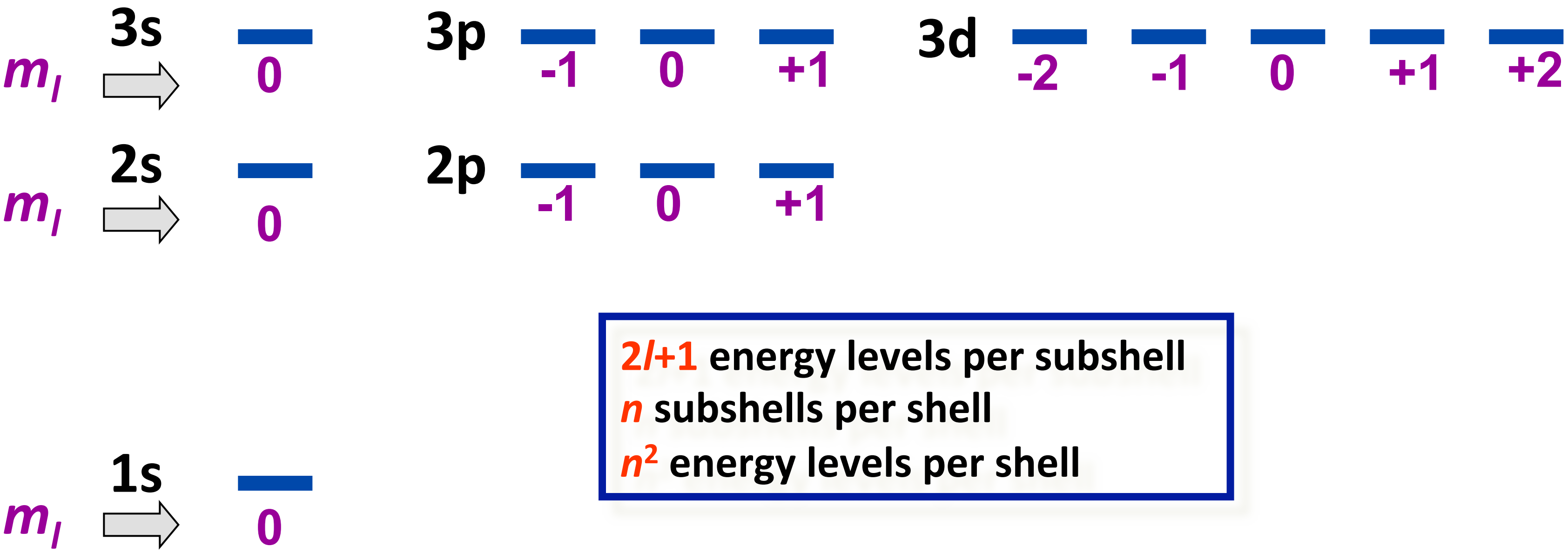
(can have a +ve or –ve value)

$\boxed{\psi^2}$ *electron density at a point in space*

(always a +ve number)

$\boxed{4\pi r^2 \psi^2}$ *probability of finding an electron at a distance r from the nucleus*

Shells, Sub-Shells & Energy Levels of H-atom

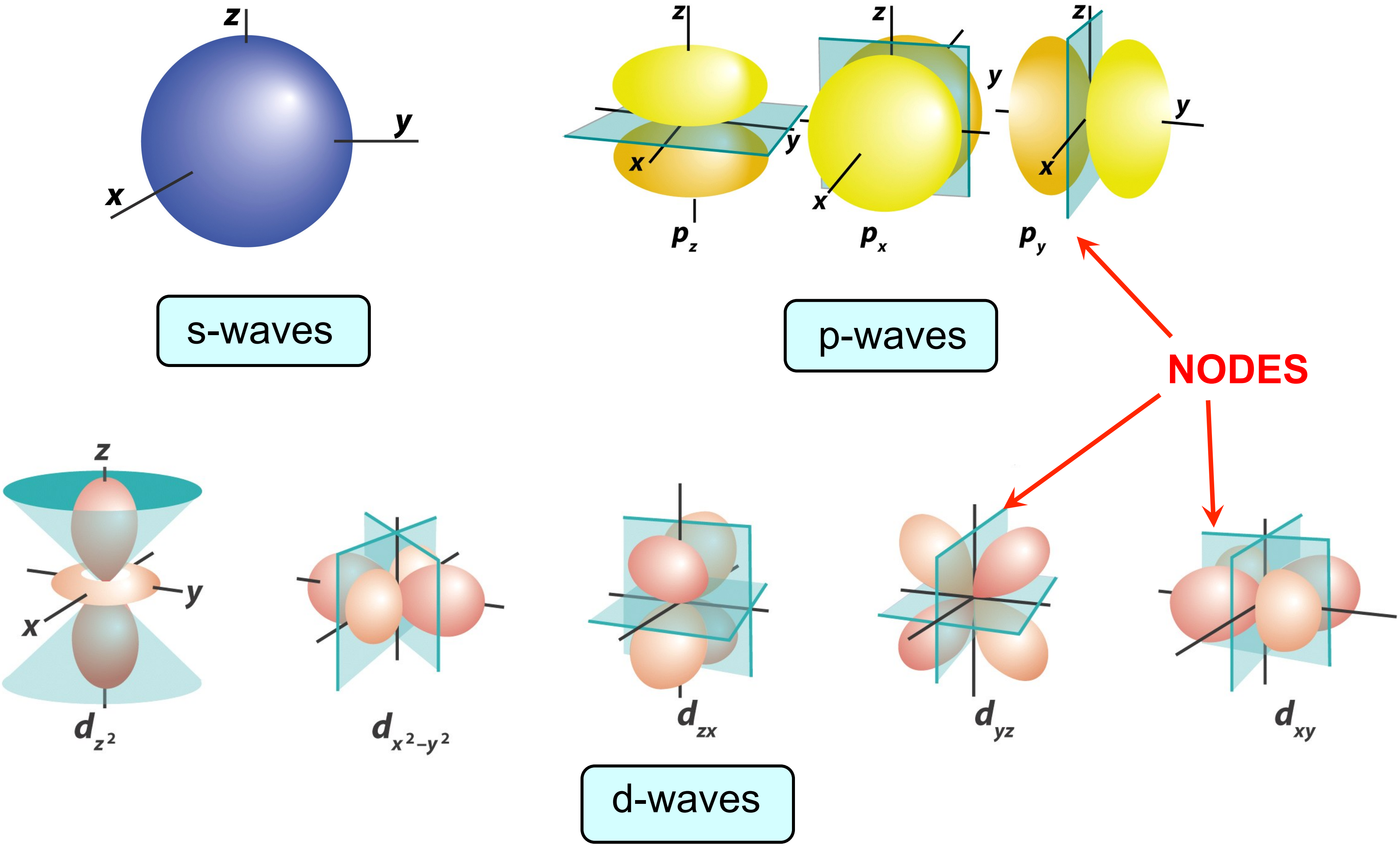


$2l+1$ energy levels per subshell
n subshells per shell
n^2 energy levels per shell

$l = 0$ ⟺ **s-orbital**
$l = 1$ ⟺ **p-orbital**
$l = 2$ ⟺ **d-orbital**
$l = 3$ ⟺ **f-orbital**

What do the Electron Waves of the H-atom look like?

Summary of Hydrogenic Orbitals



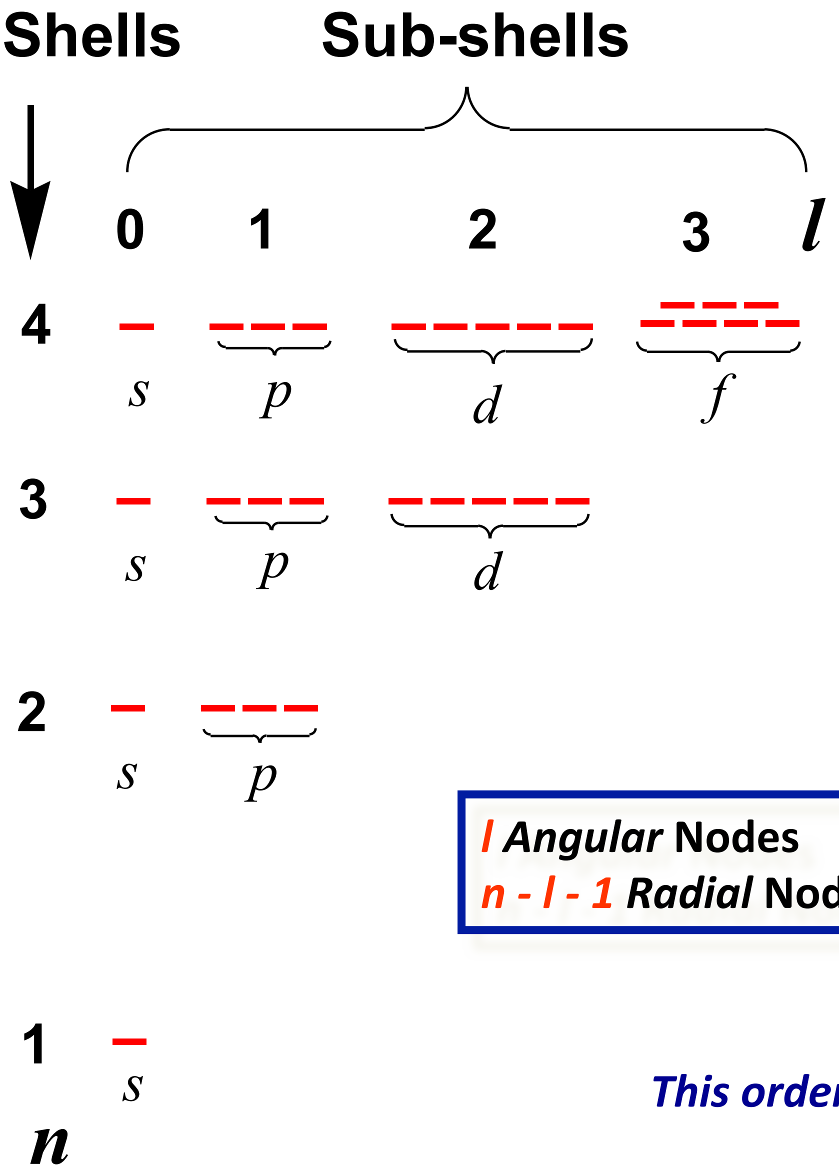
s-waves

p-waves

NODES

d-waves

Hydrogen Atom Summary



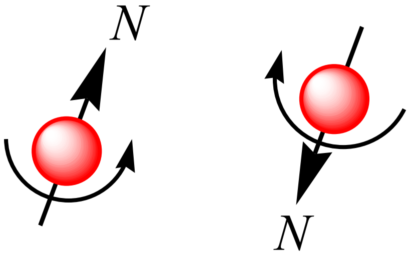
n defines energy
= 1, 2, 3, . . .

l defines orbital motion
= 0, 1, 2 . . .(n-1)

m_l defines spatial distribution
= +l to –l

m_s defines spin motion
= + ½ to – ½

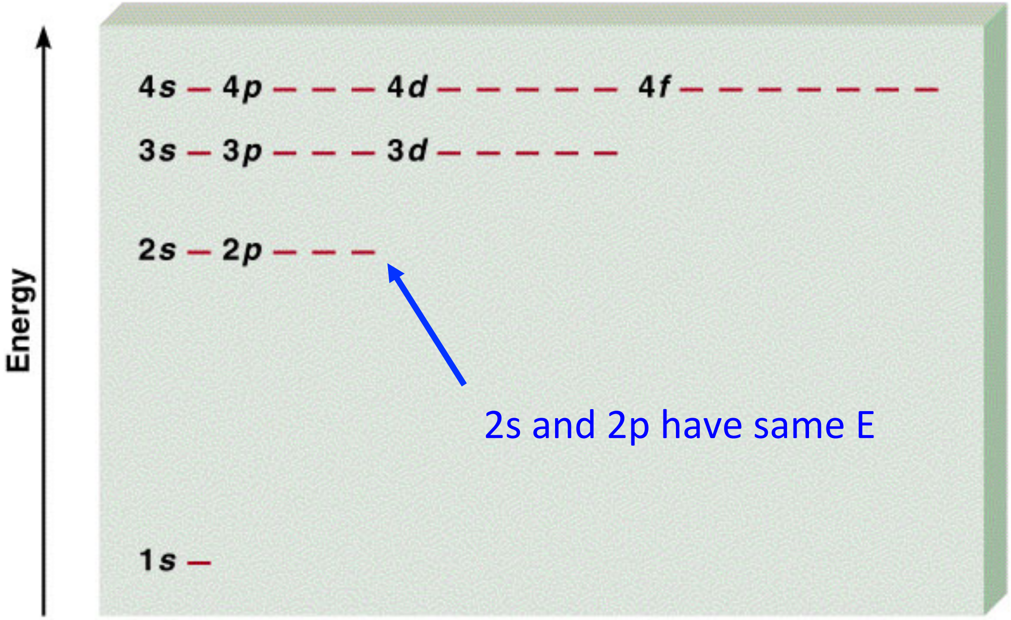
l Angular Nodes
n - l - 1 Radial Nodes



This ordering gets skewed in many electron atoms!

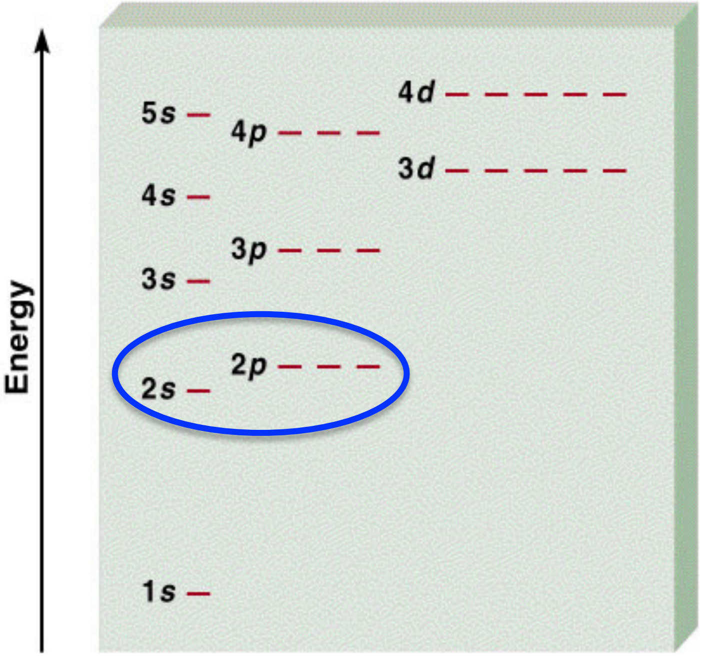
Orbital Levels in a Many Electron Atom

Hydrogen:



Orbital energies depend only on the principle quantum number, n.

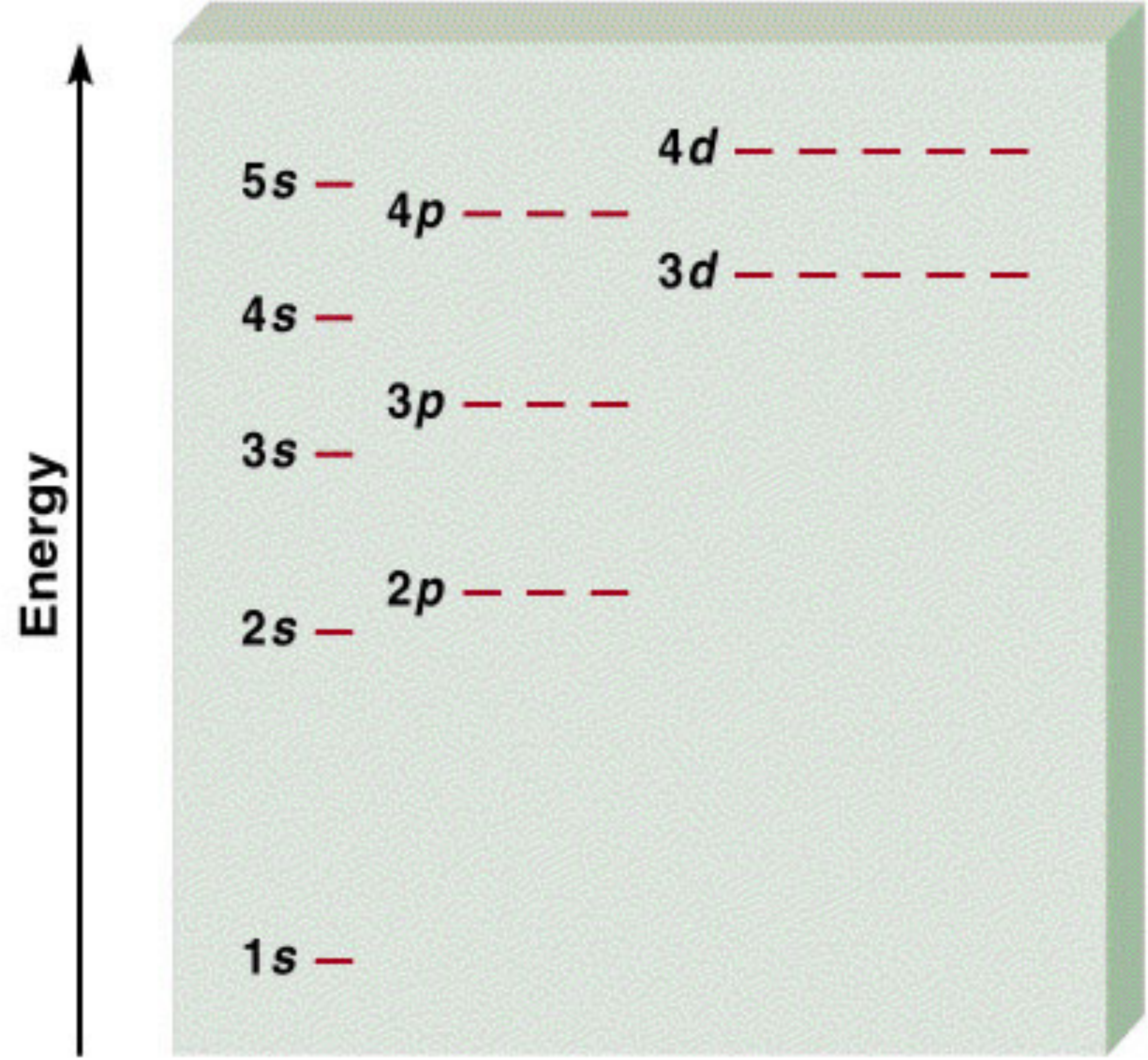
The Rest:



As a result of electron-electron repulsion, the energies of orbitals for a multi-electronic atom depend on ***both n and l***.

An electron in 2p has a higher energy (less stable) than an electron in 2s.

Orbital Levels in a Many Electron Atom



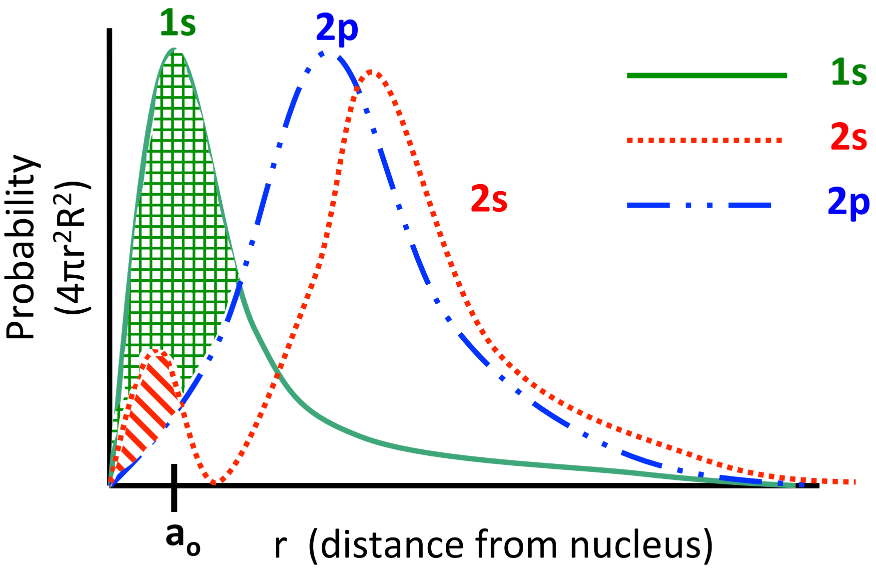
Orbital Energies in Multi-electron Atoms

Qualitative Understanding

For an electron in a given orbital:

- ➥ electron-nuclear ***attraction*** decreases (**stabilizes**) the orbital energy
- ➥ electron-electron ***repulsion*** increases (**destabilizes**) the orbital energy

Orbital Penetration



Electrons in the 1s orbital penetrate closer to the nucleus, thus ***shield*** electrons in both 2s and 2p orbitals from the attractive pull of the nucleus.

Electrons in the 2s orbital have greater penetration than 2p within the first Bohr radius (a_o), thus ***shield*** electrons in 2p orbital from the attractive pull of the nucleus.

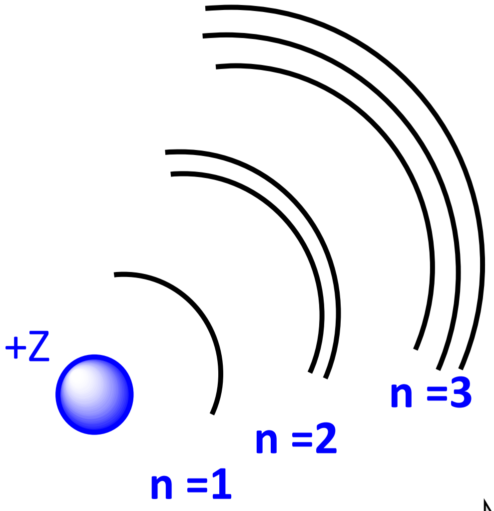
Hydrogen Atom *vs* the Rest of the Periodic Table

Hydrogen:

Nuclear charge = +1
Electron count = 1

Ground state =

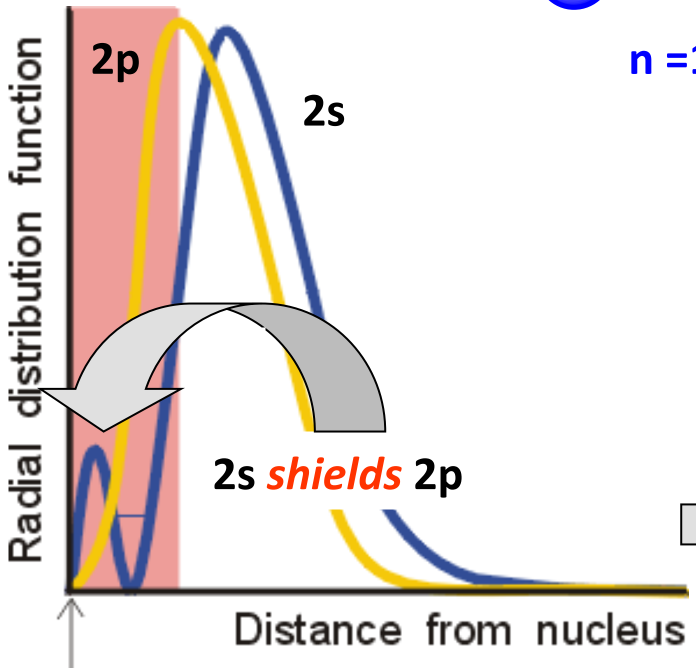
1 electron in 1s level



The Rest:

Nuclear charge = +Z
Electron count = Z

What happens to shell structure?



Nuclear charge binds electrons more tightly

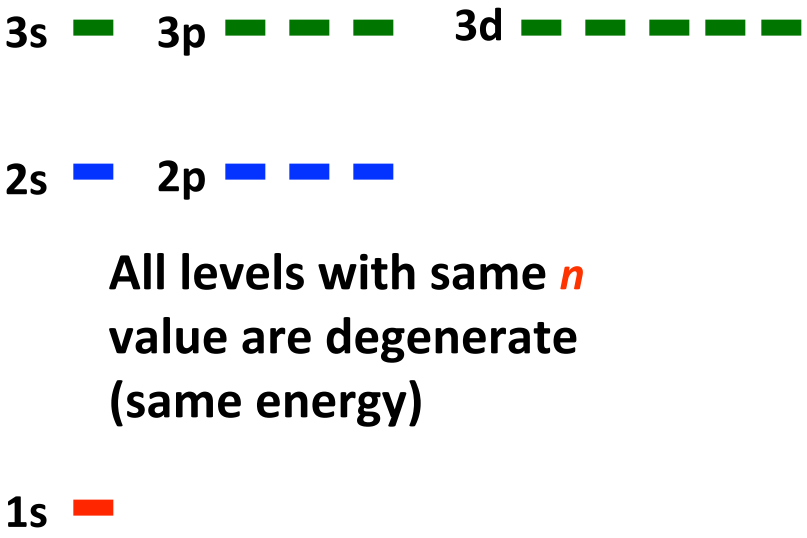
Electrons shield one another from nucleus

Subshells separate in energy

Electrons occupy lowest levels first (bottom up).

Shell Structure of Many Electron Atoms

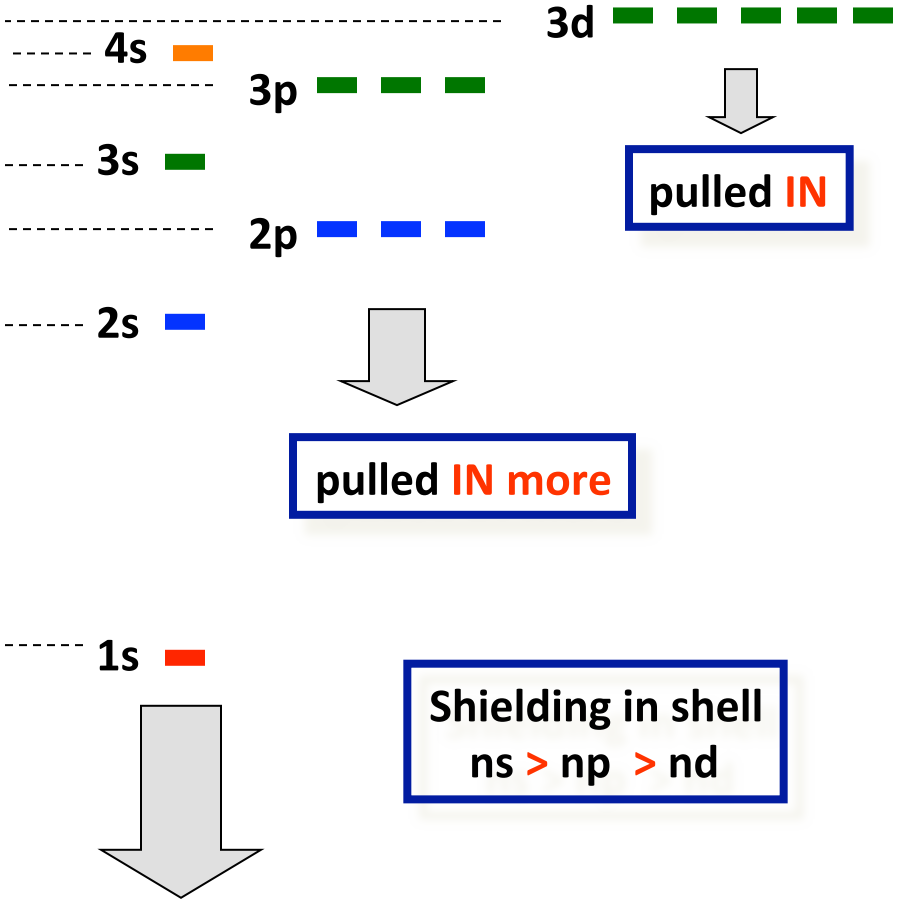
Hydrogen:



All levels with same *n* value are degenerate (same energy)

Levels with same *n* are *no longer* degenerate (same energy)

The Rest:



pulled IN

pulled IN more

pulled IN most

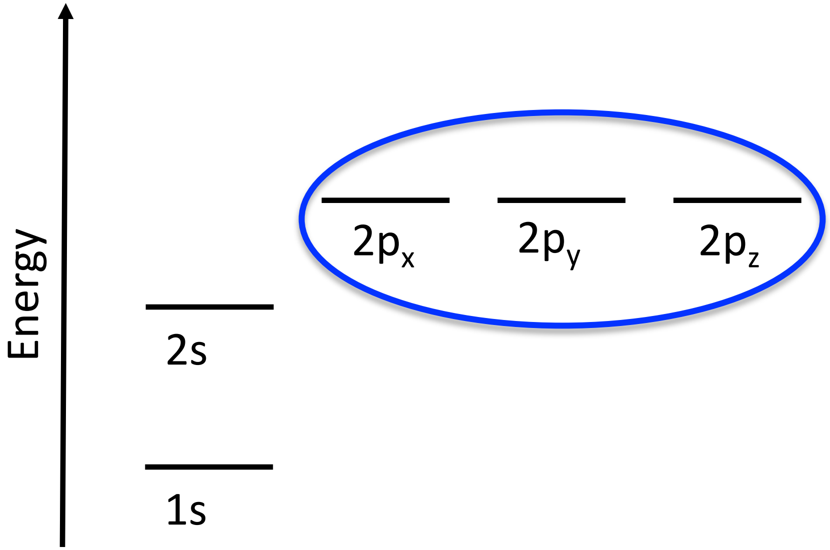
Shielding in shell
ns > np > nd

Orbital Penetration

In multi-electron atoms, orbital penetration and shielding results in the following:

Relative attraction to nucleus: 1s > 2s > 2p

Relative orbital energy: 1s < 2s < 2p



$2p_x$, $2p_y$, and $2p_z$ still have identical energies

Electron Configurations

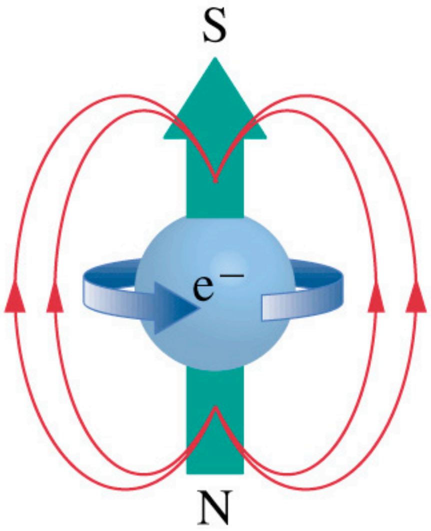
The ***Electron Configuration*** for an atom illustrates how the electrons are distributed among the various orbitals.

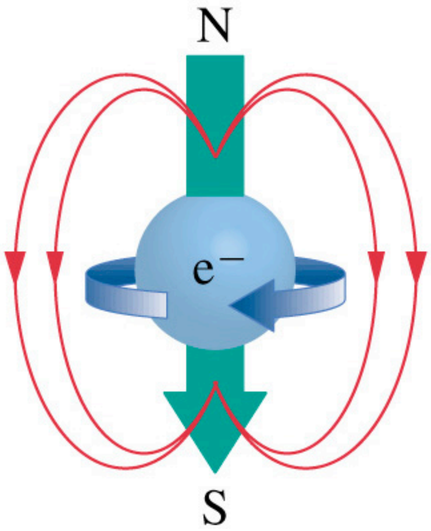
Rules:

1) Pauli Exclusion Principle
2) Aufbau Principle
3) Hund's Rule

Enter the 4th Quantum Number: Electron Spin, m_s

$m_s = + ½$





$m_s = – ½$

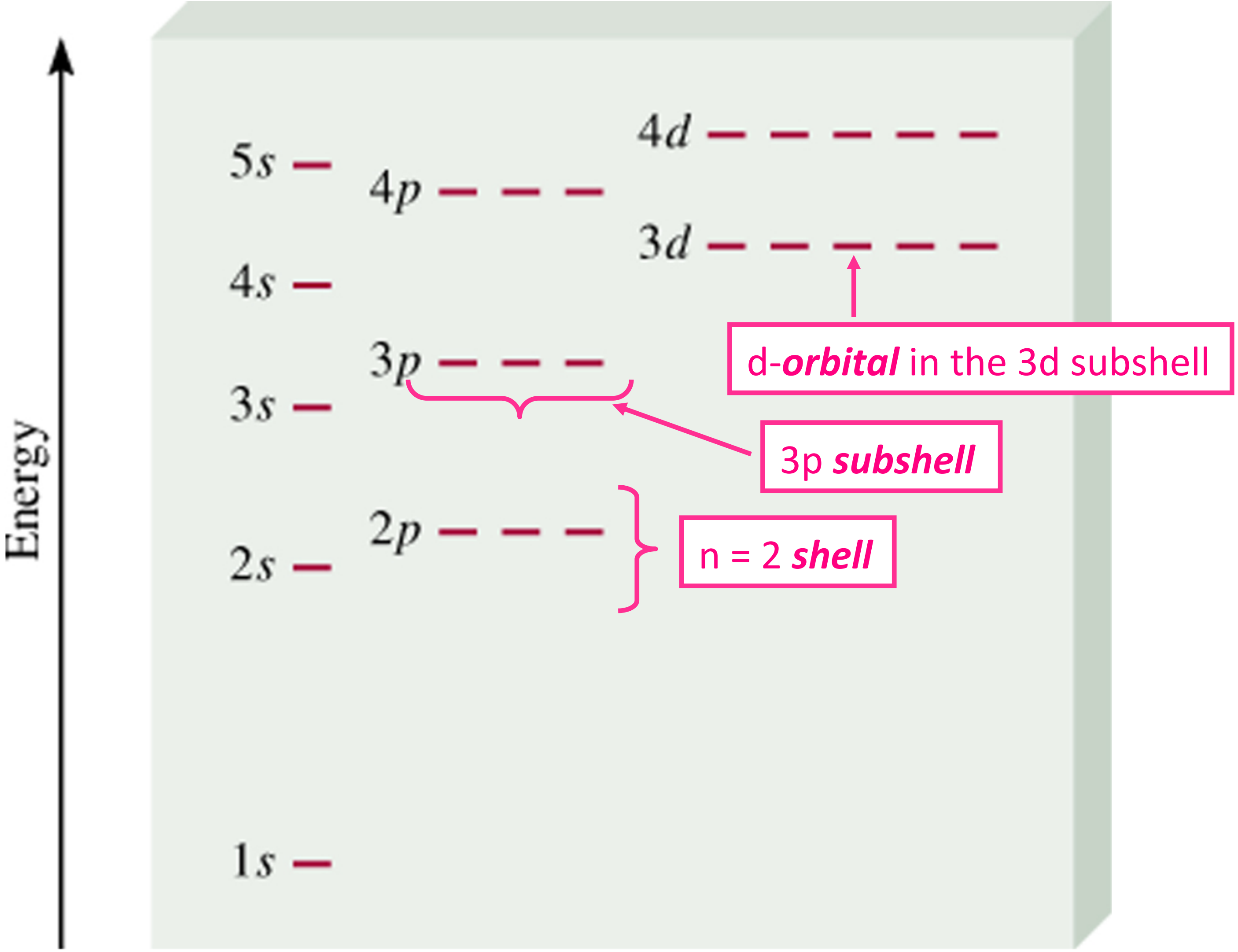
Electrons behave ***as if*** they were spinning on an axis.

Spinning charge generates a magnetic field.

Electrons can either spin clockwise or counterclockwise, so the resulting magnetic field can be either "up" or down"

This gives two values for the ***electron spin quantum number:*** + ½ or – ½

Shells, Subshells and Orbitals

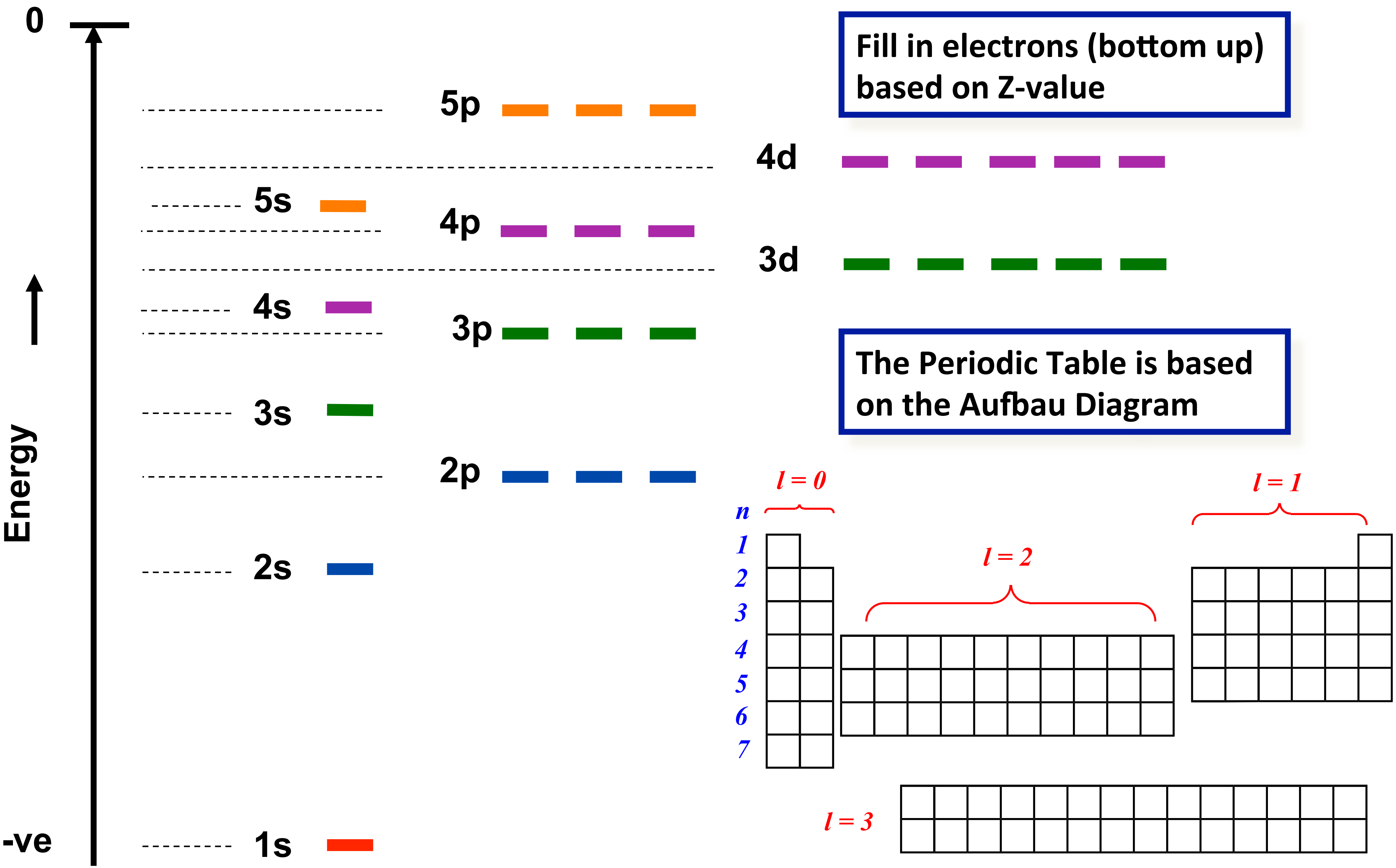


d-***orbital*** in the 3d subshell

3p ***subshell***

n = 2 ***shell***

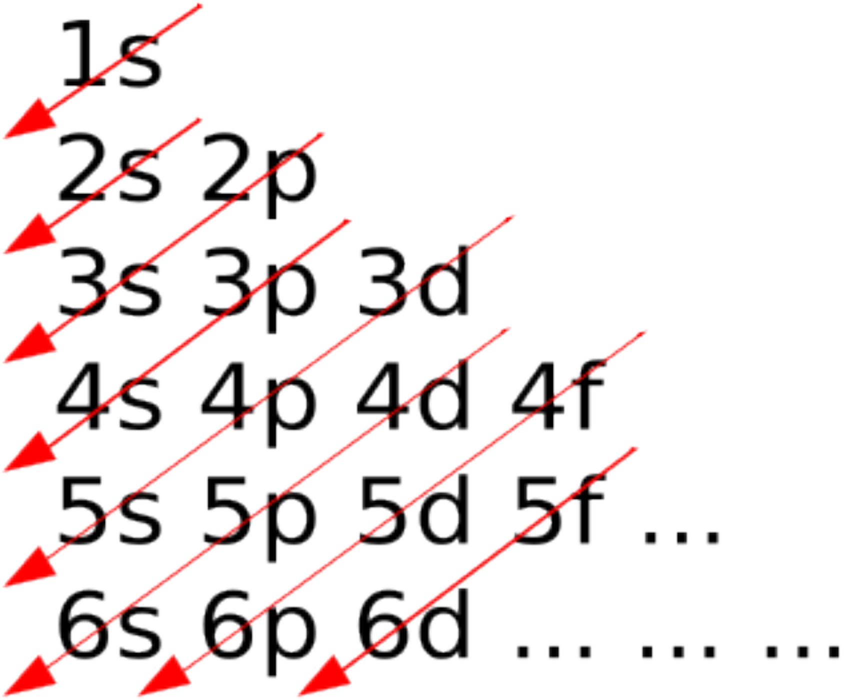
The Aufbau Diagram



Fill in electrons (bottom up) based on Z-value

The Periodic Table is based on the Aufbau Diagram

Aufbau Diagram and Electron Filling



1s

2s 2p

3s 3p 3d

4s 4p 4d 4f

5s 5p 5d 5f …

6s 6p 6d … … …

Configuration ⇨ $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$…

The Aufbau Diagram

Energy levels in most real atoms map well onto the "average" Aufbau ordering.

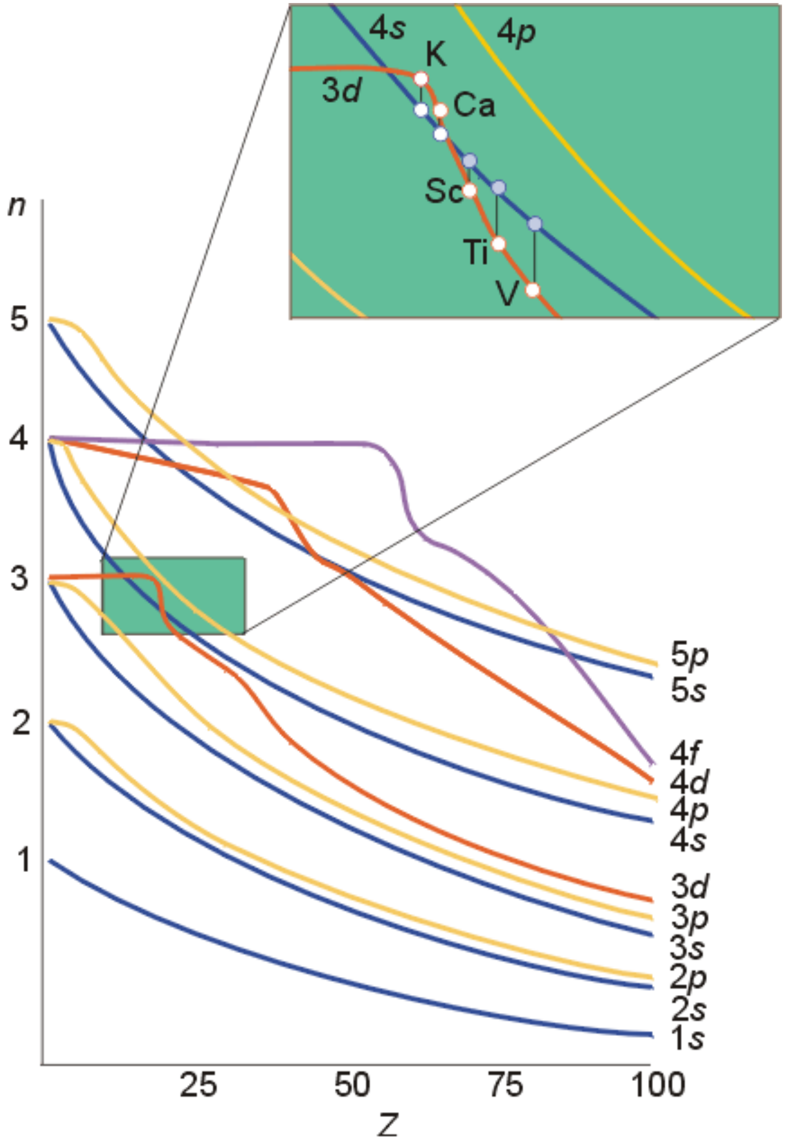
There are some wrinkles . . .

The 4s/3d levels are tricky. They wobble around a lot from element to element.

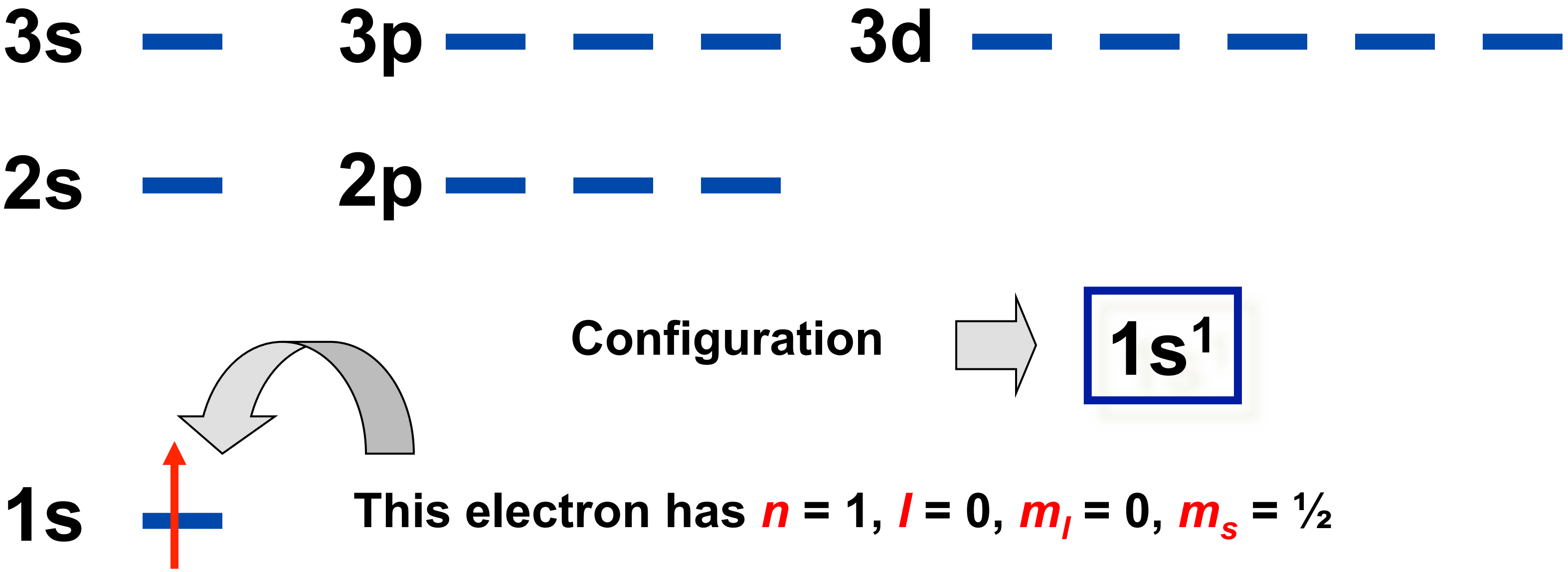
Charge on atom alters ordering.

Then there is **Hund's Rule**.

Then there is the **Pauli Principle**.



Writing Electron Configurations: Hydrogen (Z=1)



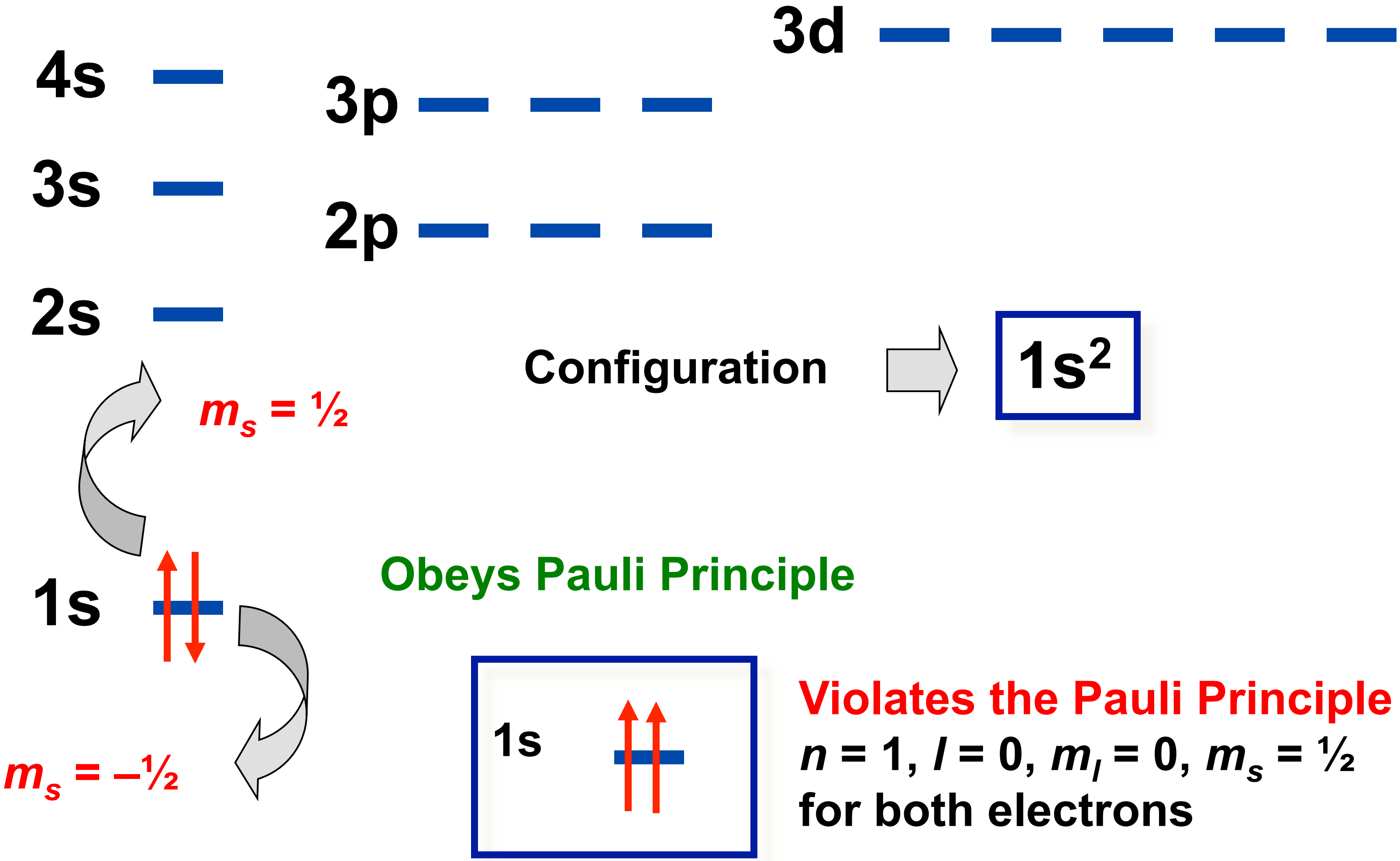
Configuration → $\boxed{1s^1}$

This electron has $n = 1$, $l = 0$, $m_l = 0$, $m_s = ½$

In Helium we could place another electron here as long as $m_s = –½$

This is the **Pauli Principle** in action. No two electrons can have the same set of quantum numbers.

Writing Electron Configurations: Helium (Z = 2)



Configuration → $\boxed{1s^2}$

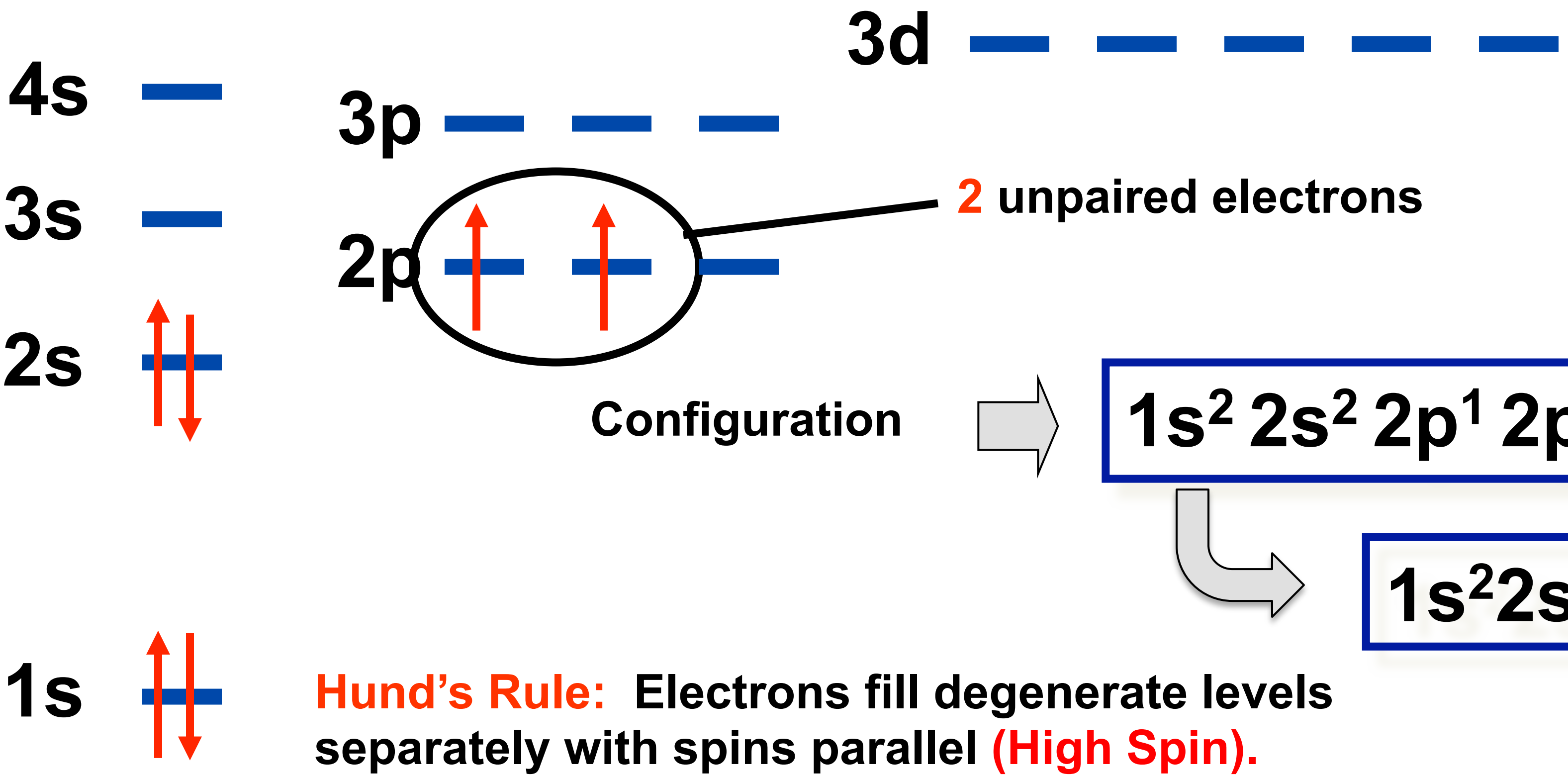
Obeys Pauli Principle

Violates the Pauli Principle

$n = 1$, $l = 0$, $m_l = 0$, $m_s = ½$

for both electrons

Writing Electron Configurations: Carbon (Z = 6)



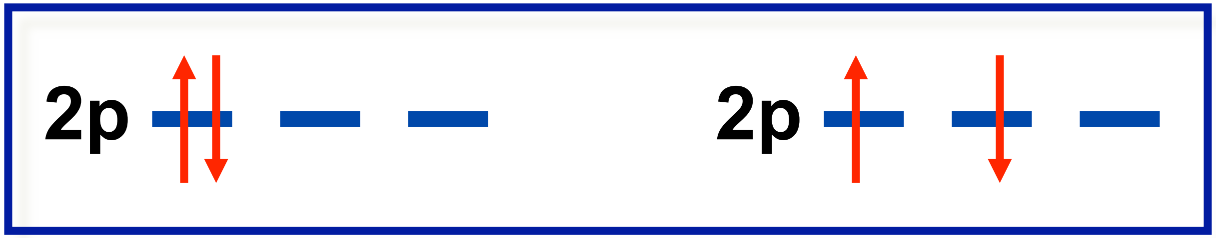
2 unpaired electrons

Configuration

$1s^2\ 2s^2\ 2p^1\ 2p^1$

$1s^22s^22p^2$

Hund's Rule: **Electrons fill degenerate levels separately with spins parallel (High Spin).**



Hund’s Rule: Why?

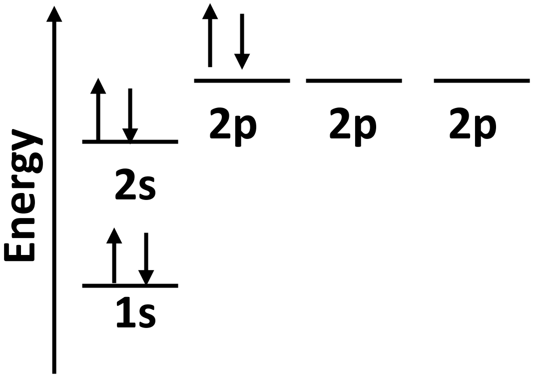
There are two energy terms that lead to Hund’s rule:

1. Coulombic Energy of Repulsion:

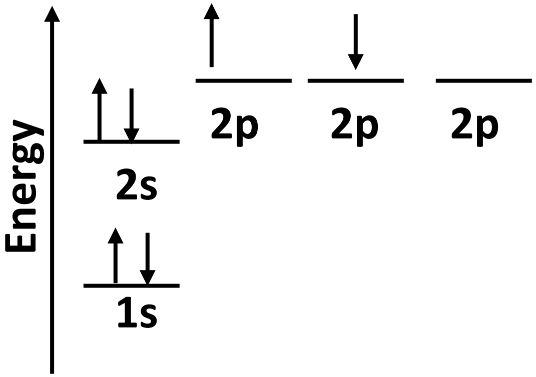
- ↳ repulsive forces between electrons cause the electrons to move into ***different*** orbitals of the ***same energy*** rather than sharing an orbital.

2. Exchange Energy:

- ↳ quantum mechanical (can’t be explained in physical terms)
- ↳ electrons in ***different*** orbitals of ***the same energy*** prefer to have the same spin
- ↳ exchange energies are negative → stabilizes high spin state

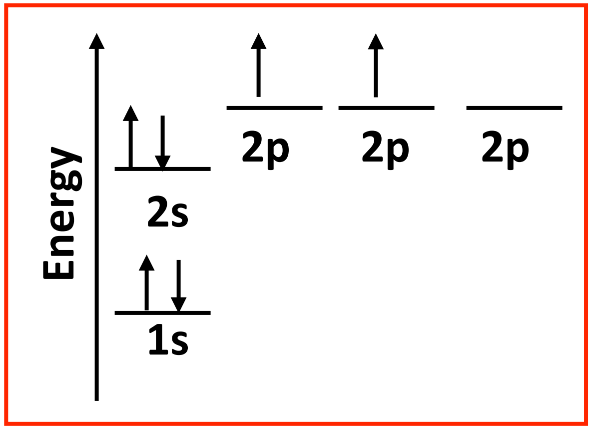


UNFAVORABLE due to Coulombic energy of repulsion.



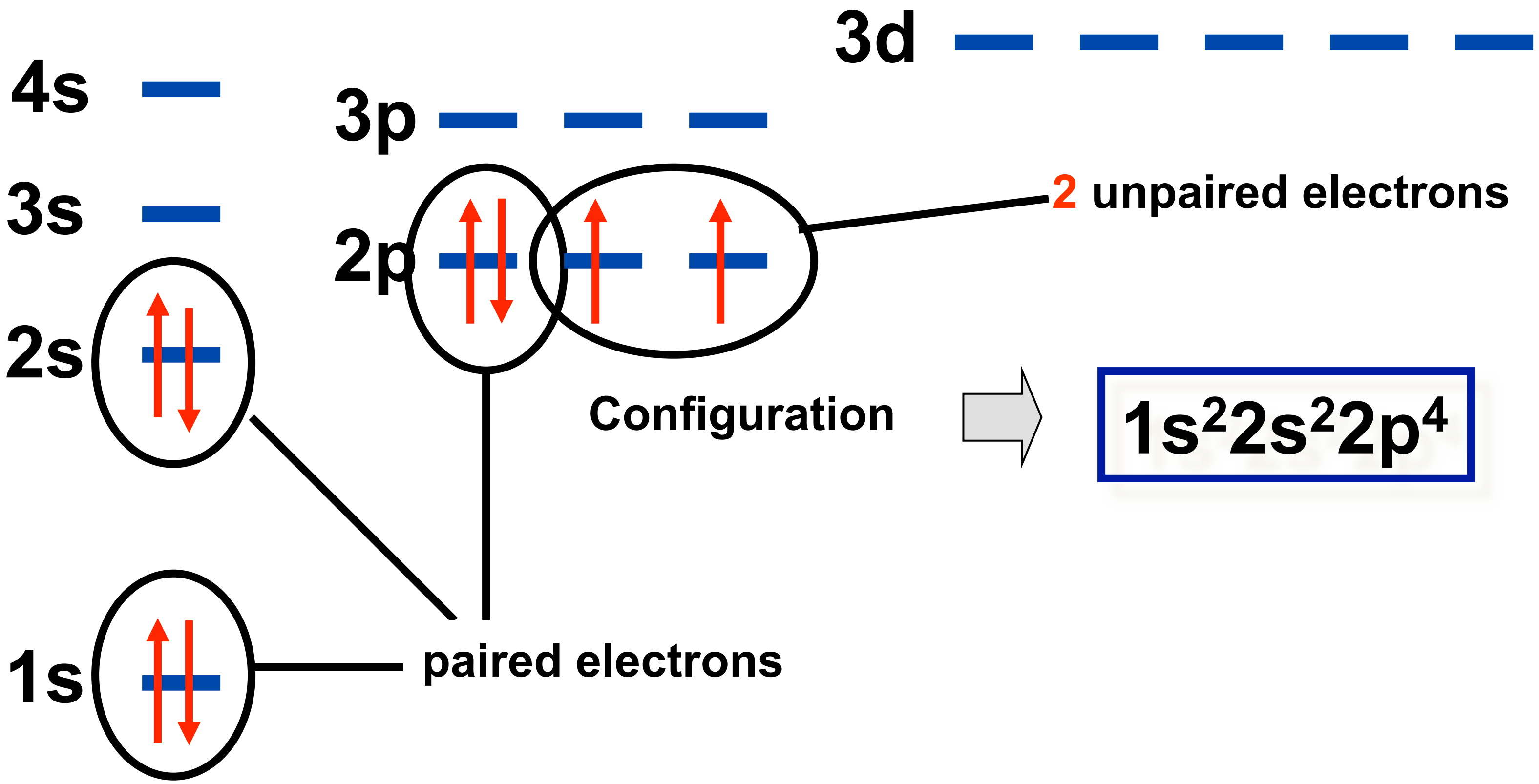
Less favorable due to exchange energy

Lowest Energy Configuration



More favorable: same spin

Writing Electron Configurations:
Oxygen (Z = 8)



2 unpaired electrons

paired electrons

Configuration → $1s^2 2s^2 2p^4$

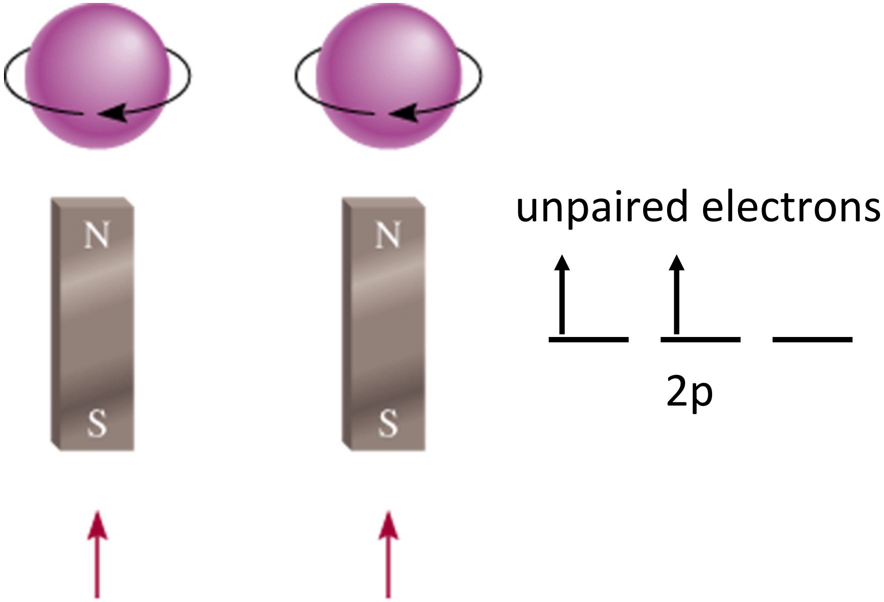
Paramagnetic → Any atom or ion with *unpaired* electrons

Diamagnetic → Any atom or ion with *all electrons paired*

Paramagnetism *vs* Diamagnetism

Paramagnetic

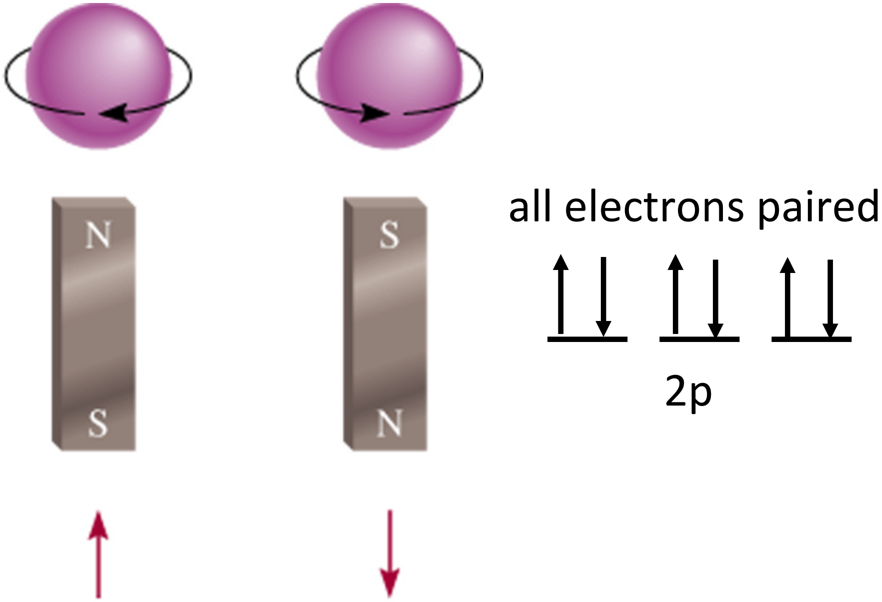
Any substance (atom, molecule, or ion) that has one or more unpaired electron.



A paramagnetic substance is attracted to a magnetic field

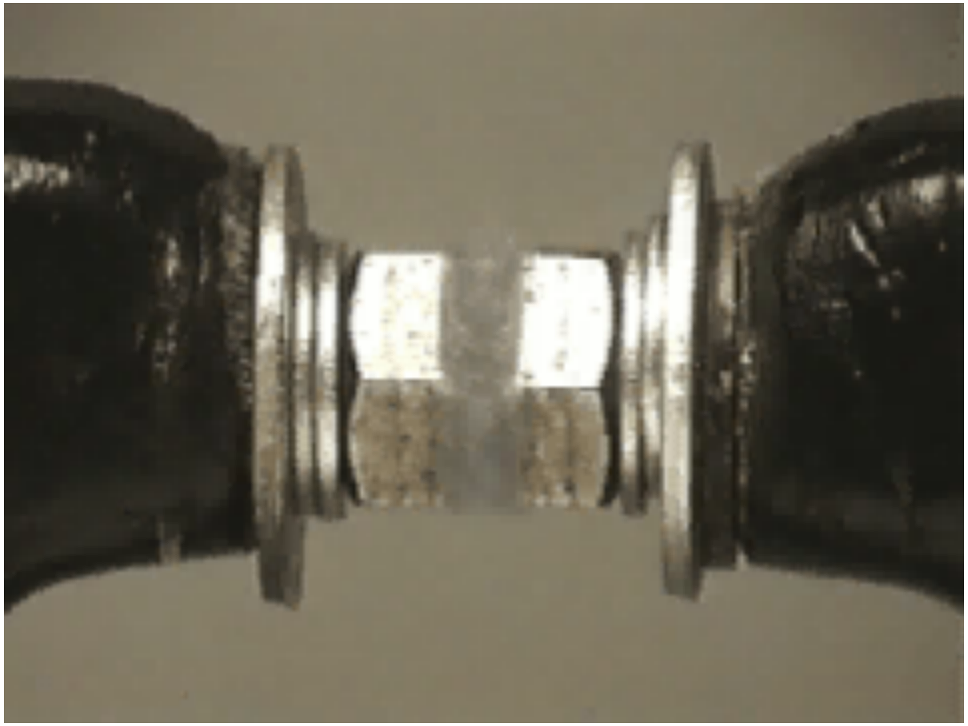
Diamagnetic

An atom, molecule, or ion that has all of its electrons paired.



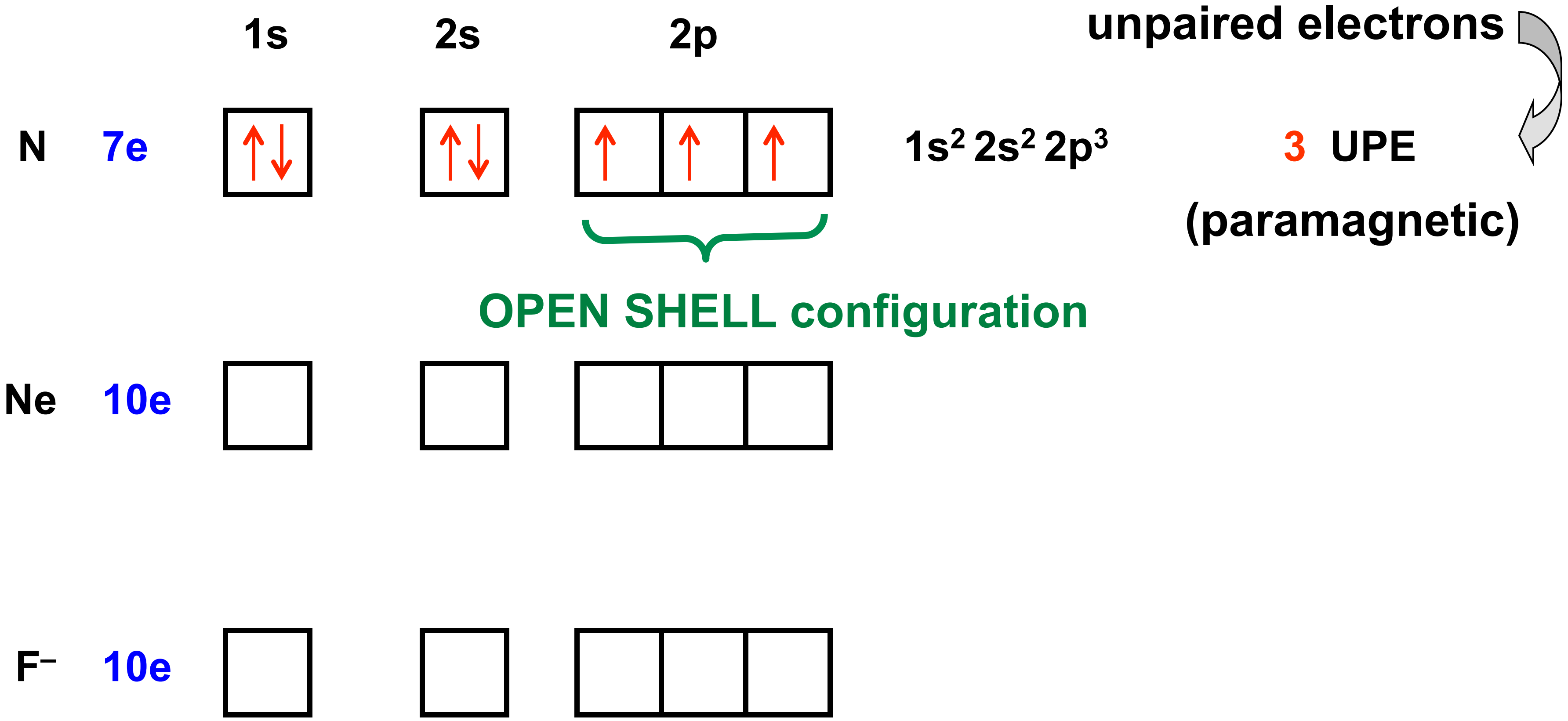
A diamagnetic substance is slightly repelled by a magnetic field

Paramagnetism *vs* Diamagnetism



Paramagnetic substances are attracted by a magnetic field.

Exercise: Fill in the Blanks…



unpaired electrons

$1s^2\,2s^2\,2p^3$

3 UPE

(paramagnetic)

OPEN SHELL configuration

Ne and F⁻ are ISOELECTRONIC

Electron Configurations:
A Summary So Far…

Pauli Exclusion Principle:

➥ *No two electrons in the same atom can have the* ***same*** *set of 4 quantum numbers.*

➥ *Each orbital can contain* ***no more than 2 electrons****:* One electron with m_s = + 1/2, and one electron with m_s = -1/2

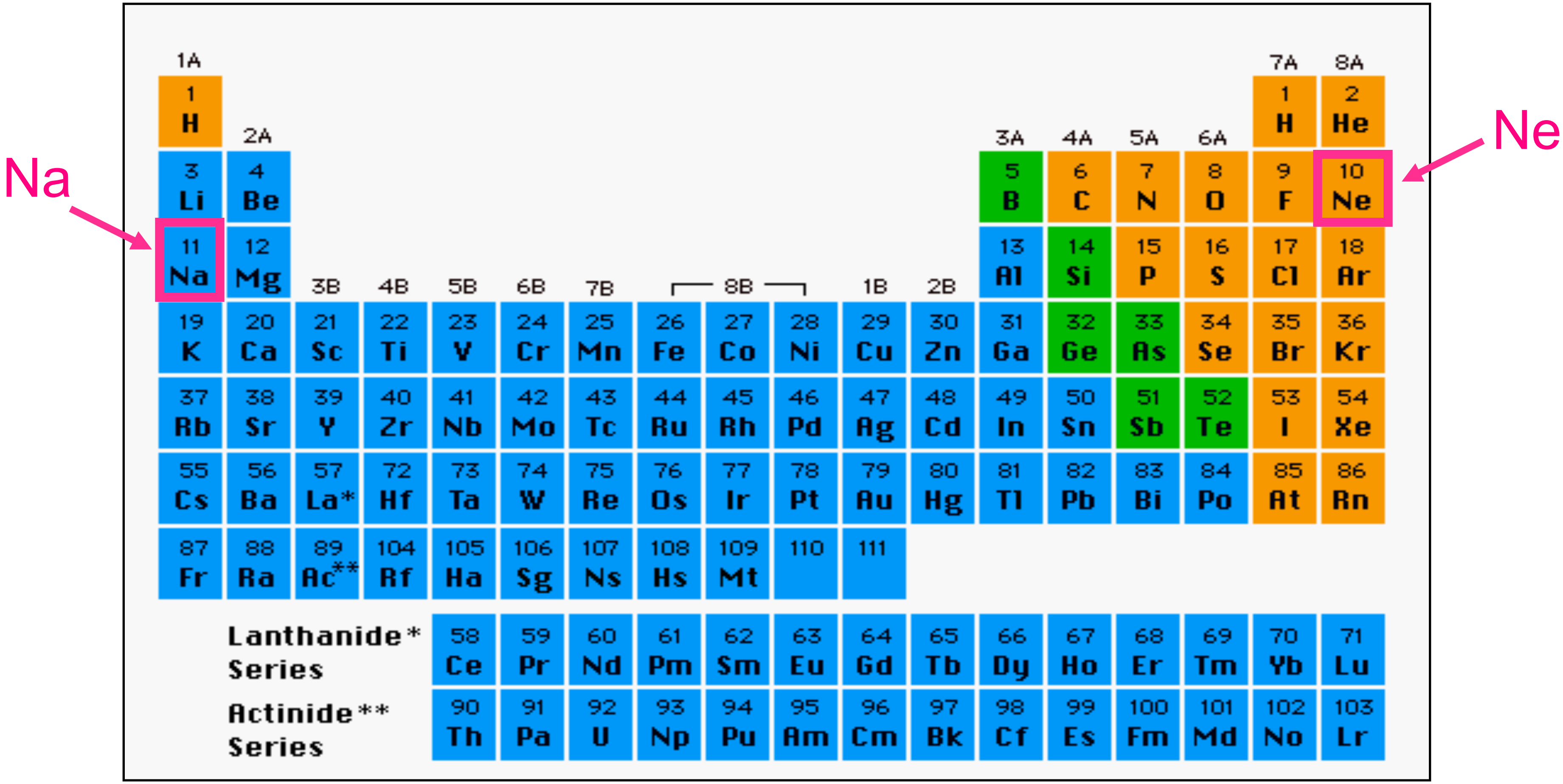
Aufbau Principle:

➥ Electrons in an atom in the ground state will occupy the orbitals of ***lowest*** energy.

Hund's Rule:

➥ When placing electrons in a set of orbitals having the same energy, the number of unpaired electrons will be ***maximized*** and will have parallel spins.

Noble Gas Core Representation



1A	2A	3B	4B	5B	6B	7B	8B			1B	2B	3A	4A	5A	6A	7A	8A
1 H																1 H	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
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
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
55 Cs	56 Ba	57 La*	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
87 Fr	88 Ra	89 Ac**	104 Rf	105 Ha	106 Sg	107 Ns	108 Hs	109 Mt	110	111							
	Lanthanide* Series			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
	Actinide** Series			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

Electron Configuration of Na: $1s^2\ 2s^2\ 2p^6\ 3s^1$

Electron Configuration of Ne: $1s^2\ 2s^2\ 2p^6$

Noble Gas Core Representation of Na: $[Ne]\ 3s^1$

Noble Gas Core Representation

The inner core of electrons is represented by the symbol for the corresponding noble gas in brackets.

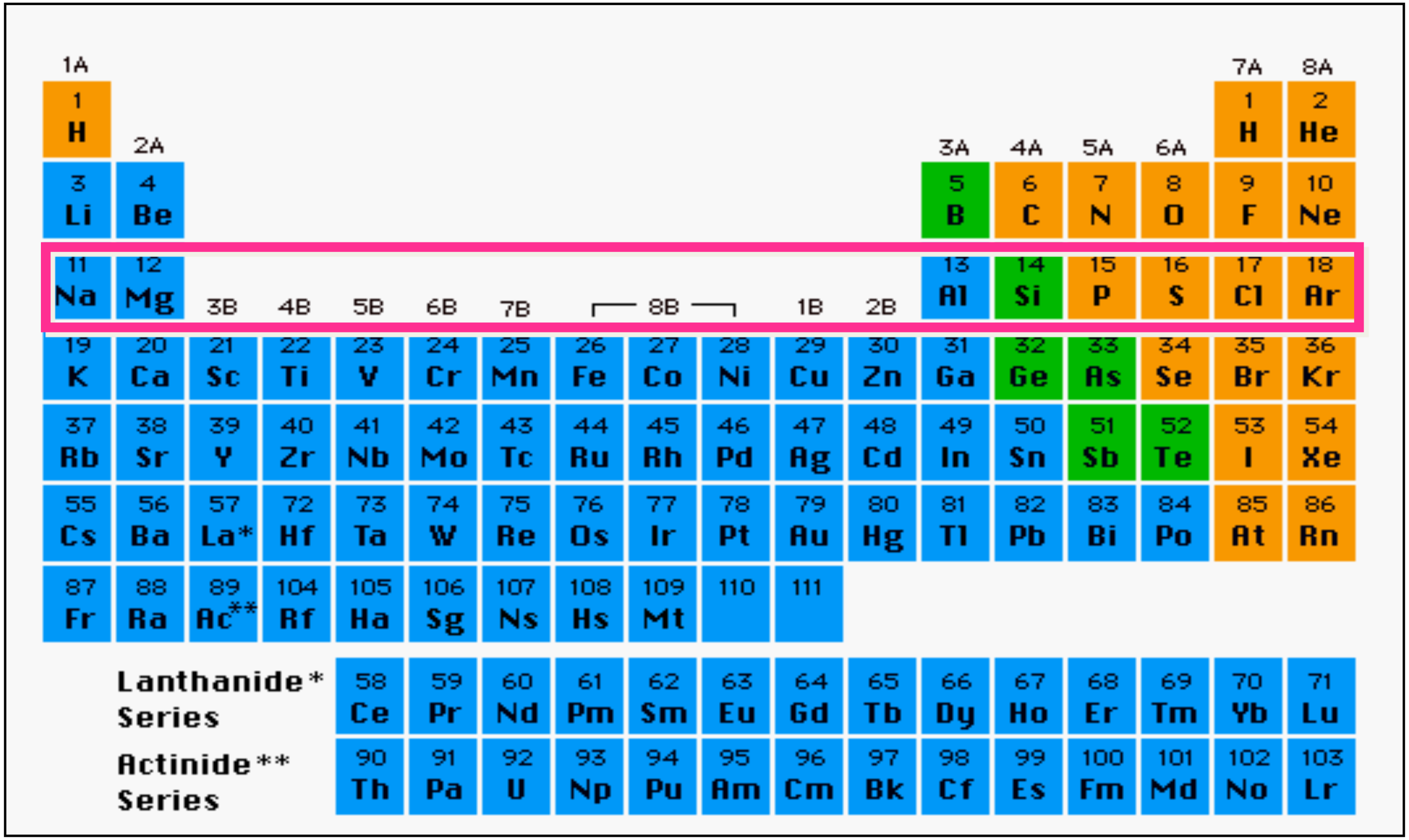
Silicon: $1s^2\ 2s^2\ 2p^6\ 3s^2 3p^2$

Neon: $1s^2\ 2s^2\ 2p^6$

Noble gas core representation of Si: $[\mathrm{Ne}]3s^2 3p^2$

The "noble gas core" will always be the noble gas that most ***immediately precedes*** the element of interest.

Electron Configurations for Period 3



1A	2A	3B	4B	5B	6B	7B	8B	8B	8B	1B	2B	3A	4A	5A	6A	7A	8A
1 H																1 H	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
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
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
55 Cs	56 Ba	57 La*	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
87 Fr	88 Ra	89 Ac**	104 Rf	105 Ha	106 Sg	107 Ns	108 Hs	109 Mt	110	111							
	Lanthanide* Series			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
	Actinide** Series			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

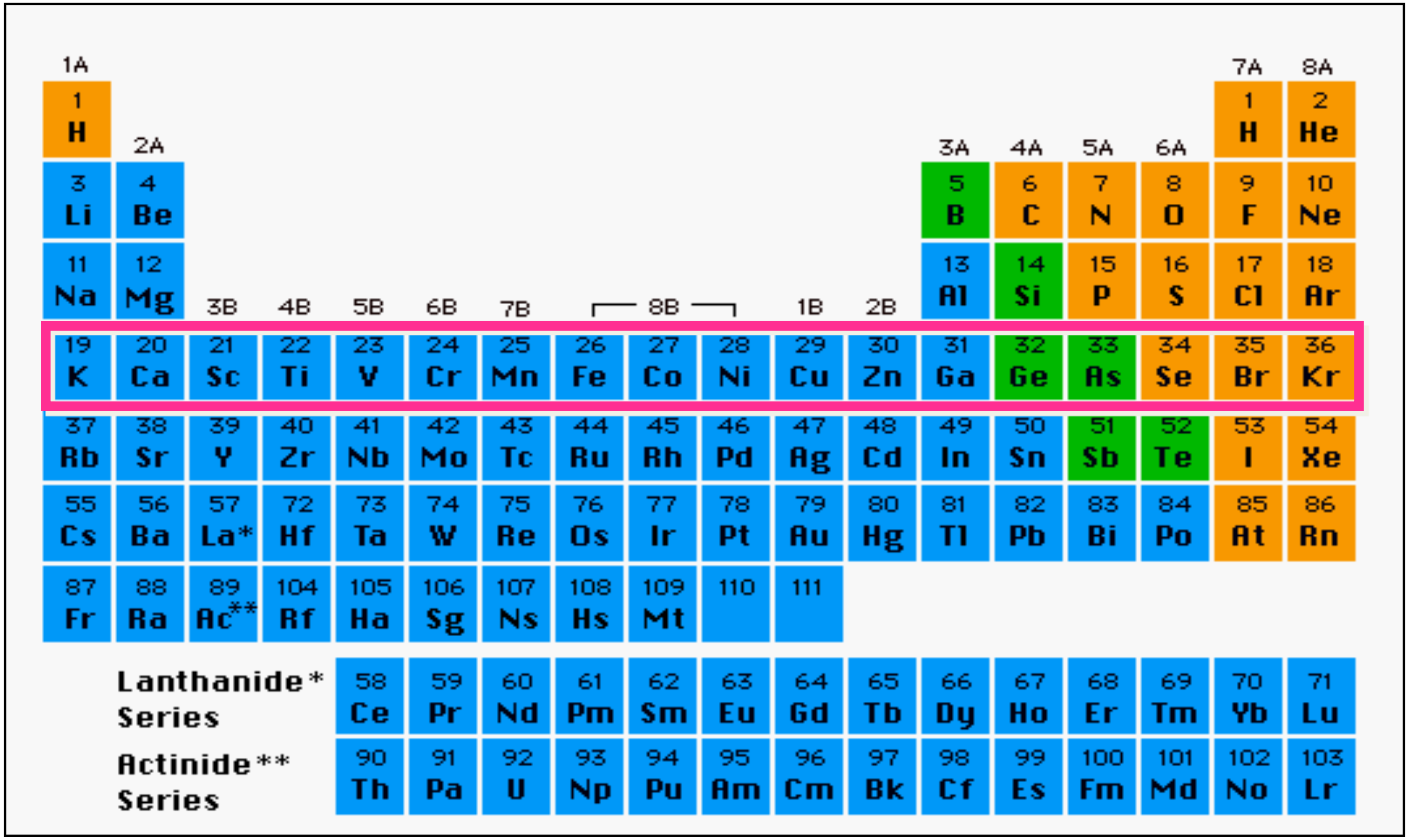
Na: [Ne] $3s^1$
Mg: [Ne] $3s^2$

Al: [Ne] $3s^23p^1$
Si: [Ne] $3s^23p^2$

P: [Ne] $3s^23p^3$
S: [Ne] $3s^23p^4$

Cl: [Ne] $3s^23p^5$
Ar: [Ne] $3s^23p^6$

Electron Configurations for Period 4



1A																7A	8A
1 H	2A											3A	4A	5A	6A	1 H	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg	3B	4B	5B	6B	7B	8B			1B	2B	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
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
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
55 Cs	56 Ba	57 La*	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
87 Fr	88 Ra	89 Ac**	104 Rf	105 Ha	106 Sg	107 Ns	108 Hs	109 Mt	110	111							
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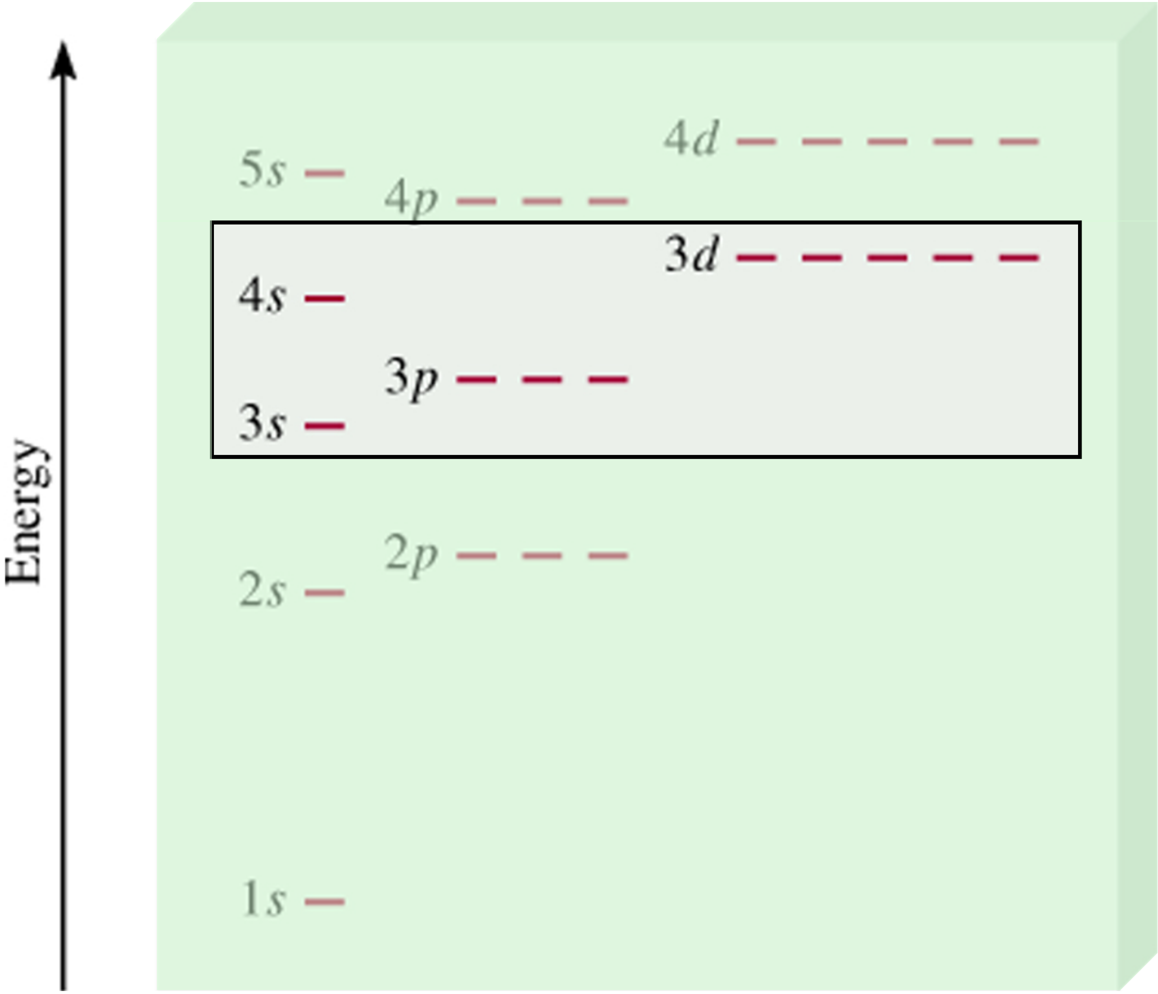
	Actinide** Series			90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

K: [Ar]$4s^1$ Ca: [Ar]$4s^2$

What is the electron configuration of Scandium???

Electron Configurations for Period 4

Aufbau Principle Revisited:

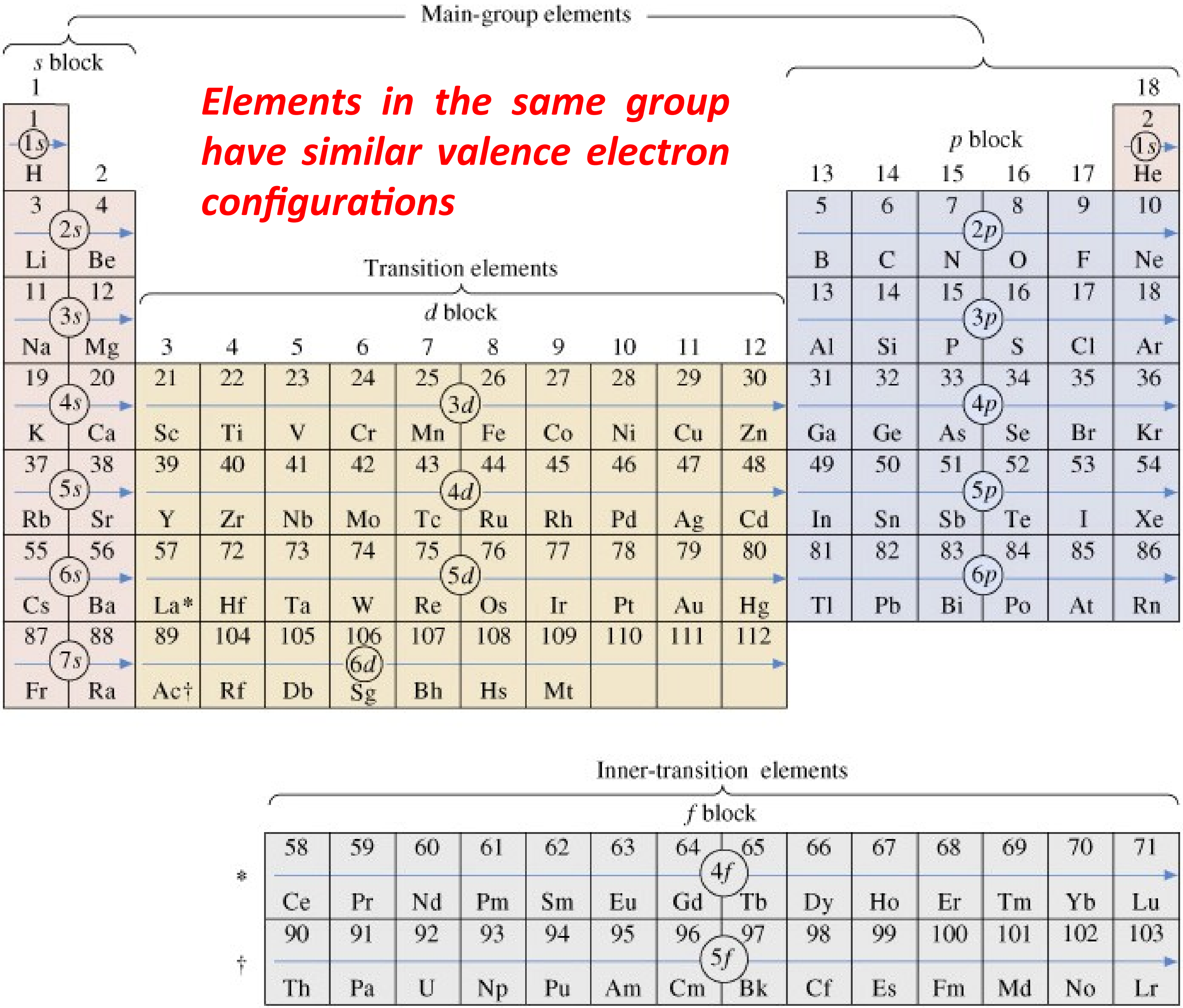


The 3 d-orbitals are filled *after* the 4 s-orbitals!

Ca: 20 electrons ⇨ [Ar]$4s^2$

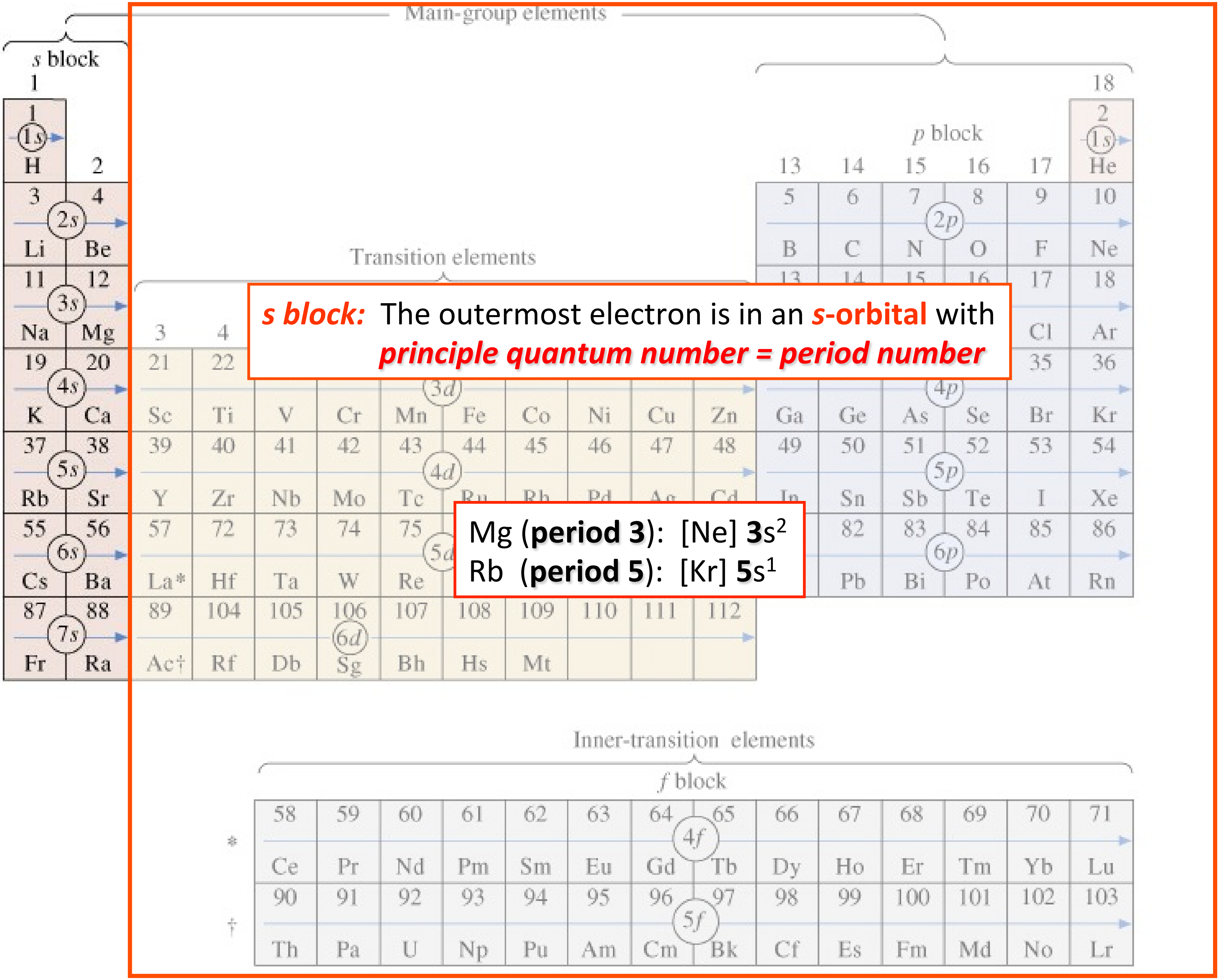
Sc: 21 electrons ⇨ [Ar]$4s^2$**$3d^1$**

Elements in the same group have similar valence electron configurations



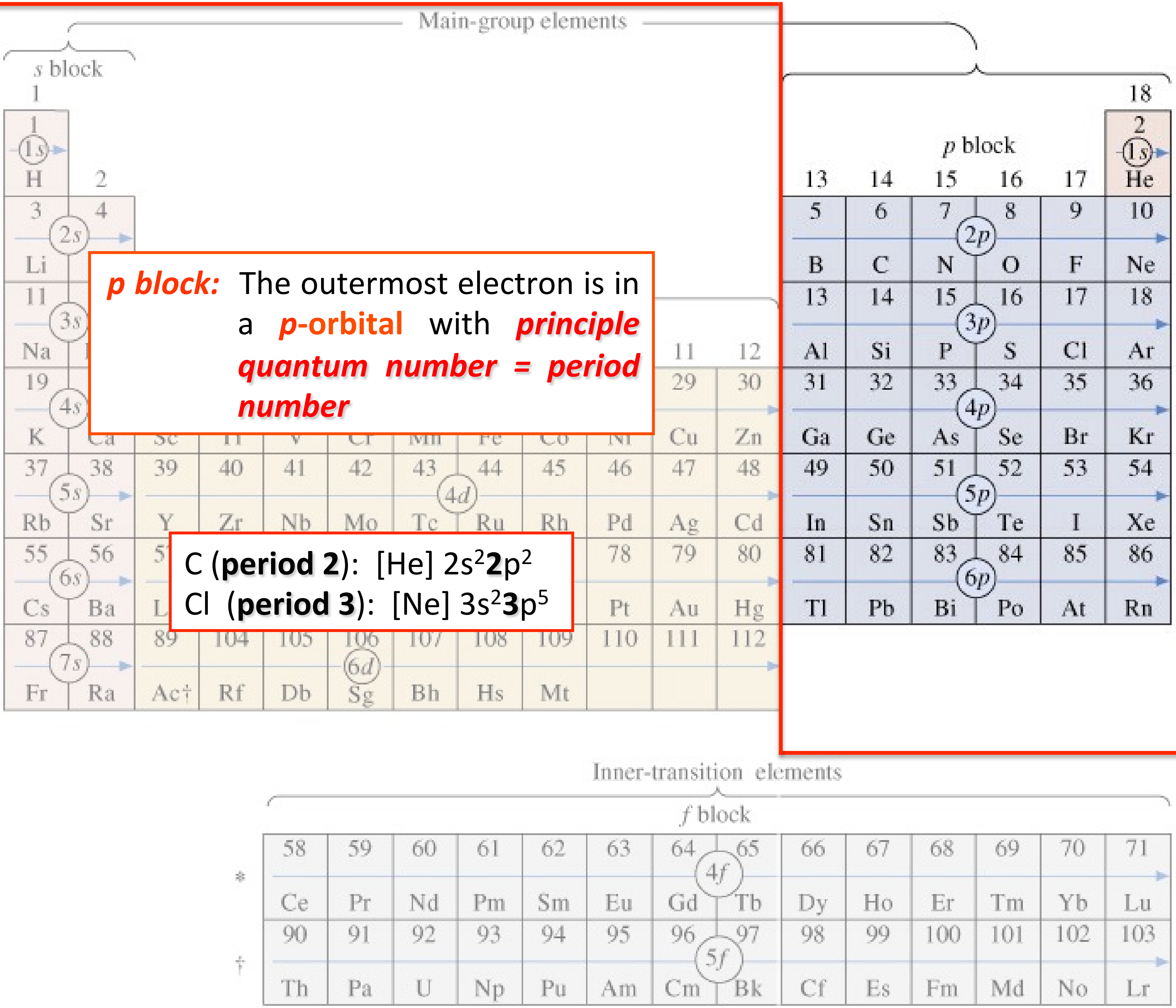
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	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
55 Cs	56 Ba	57 La*	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
87 Fr	88 Ra	89 Ac†	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110	111	112						

*	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
†	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



s block: The outermost electron is in an ***s*-orbital** with ***principle quantum number = period number***

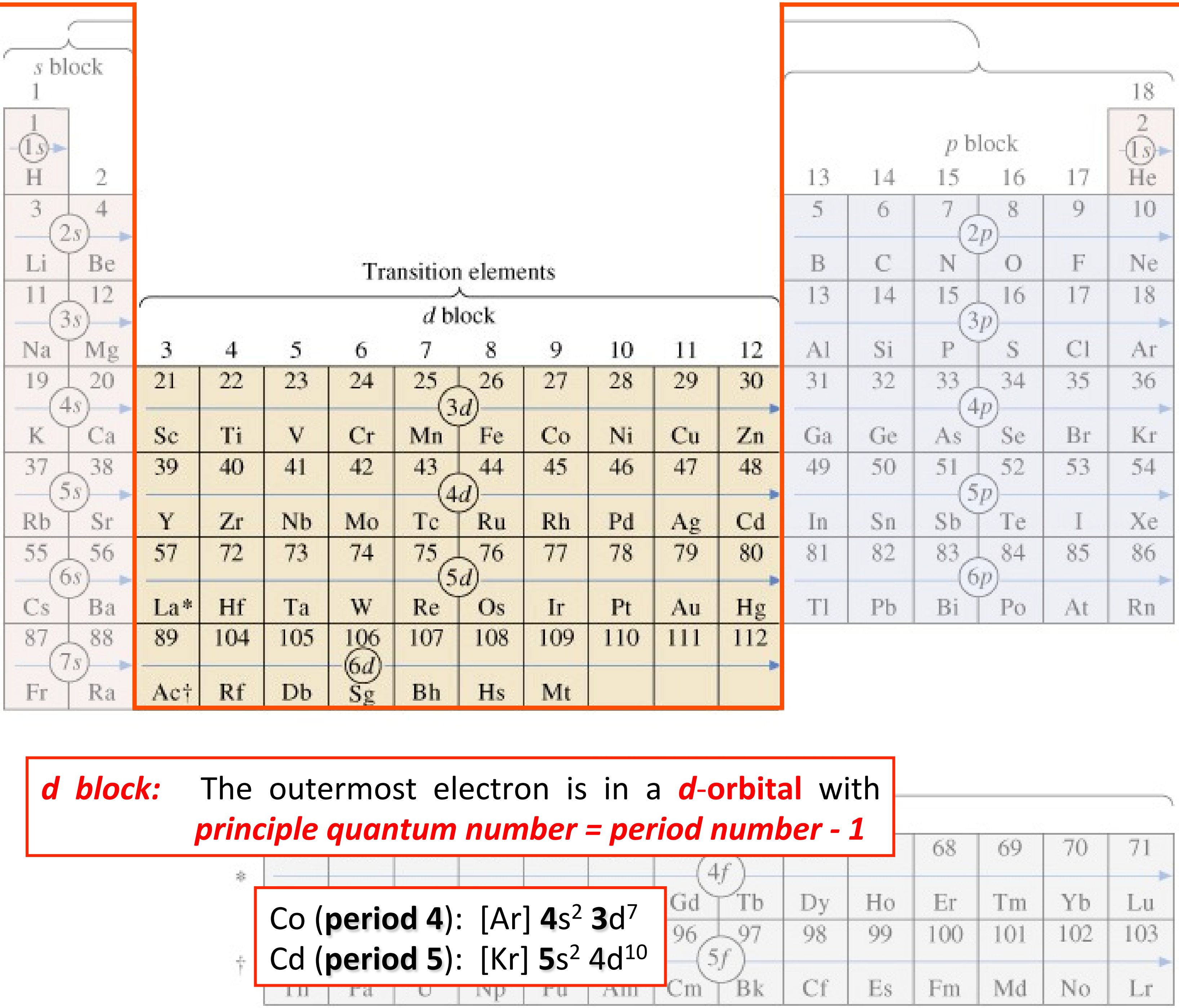
Mg (**period 3**): [Ne] **3**s^2
Rb (**period 5**): [Kr] **5**s^1



p block: The outermost electron is in a ***p-orbital*** with ***principle quantum number = period number***

C (**period 2**): [He] $2s^2\mathbf{2}p^2$

Cl (**period 3**): [Ne] $3s^2\mathbf{3}p^5$



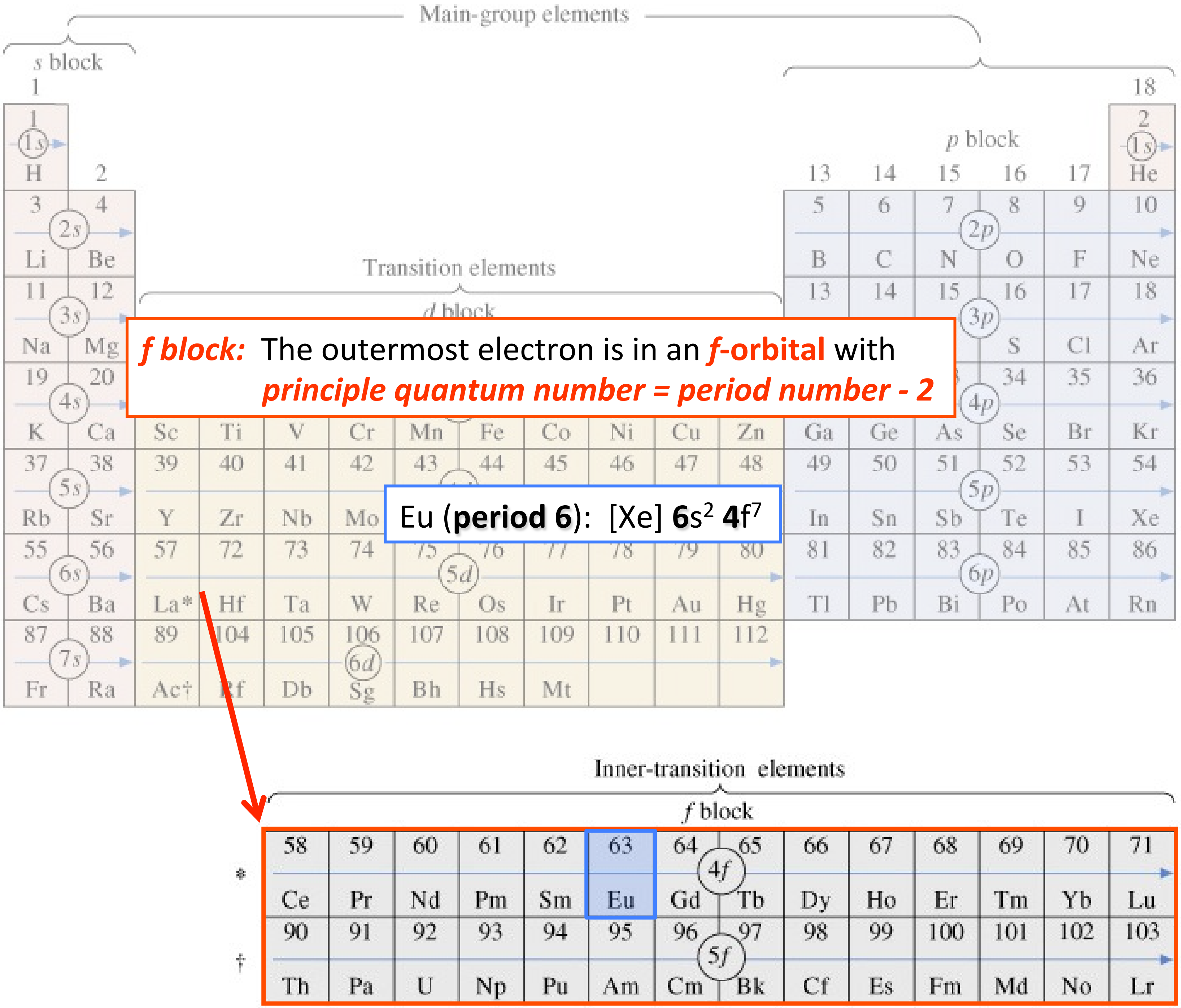
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	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
55 Cs	56 Ba	57 La*	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
87 Fr	88 Ra	89 Ac†	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110	111	112						

*	Gd	Tb	Dy	Ho	68 Er	69 Tm	70 Yb	71 Lu
†	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

d block: The outermost electron is in a ***d*-orbital** with ***principle quantum number = period number - 1***

Co (**period 4**): [Ar] **4**s^2 **3**d^7

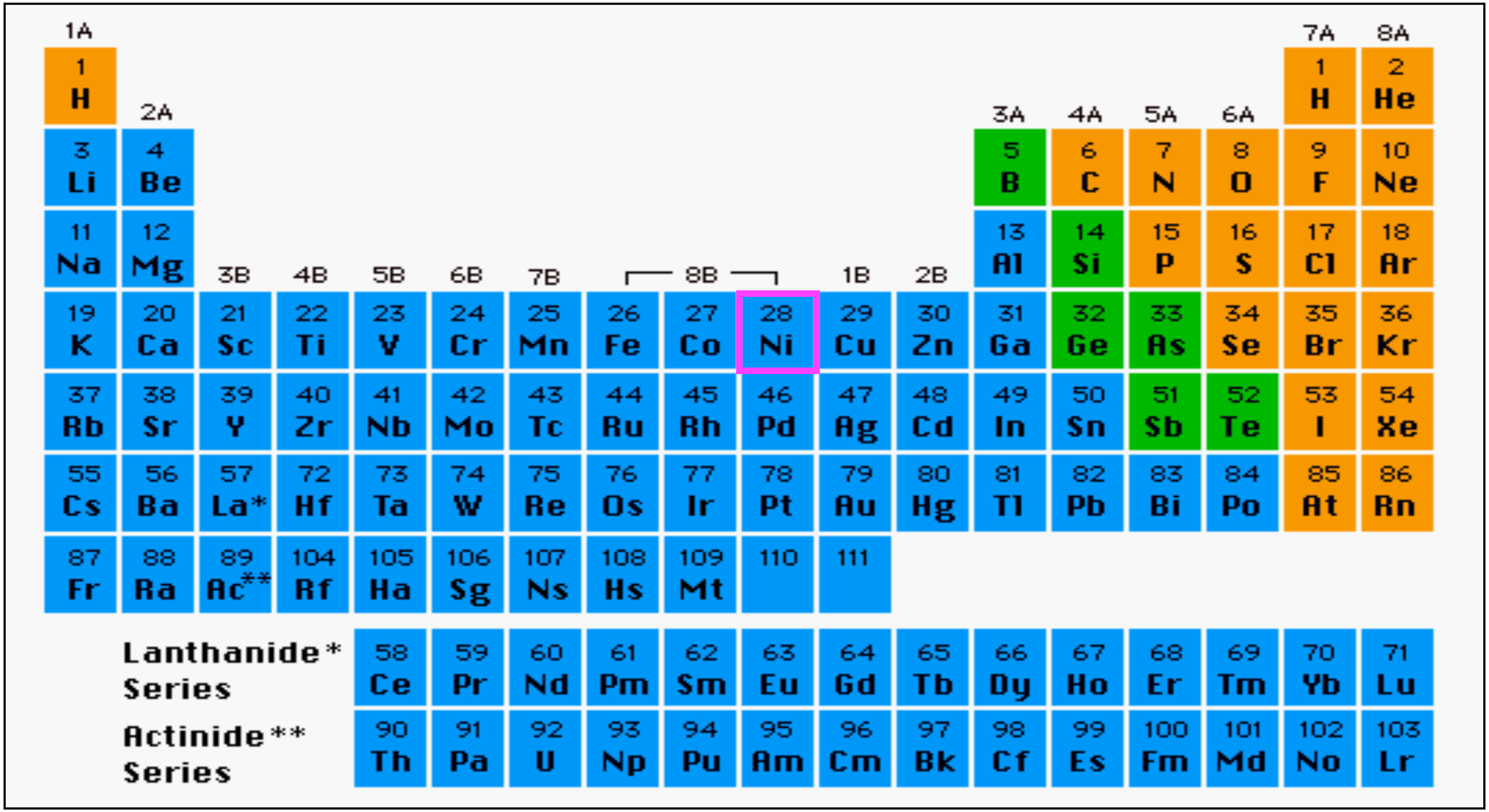
Cd (**period 5**): [Kr] **5**s^2 4d^{10}



f block: The outermost electron is in an ***f*-orbital** with
principle quantum number = period number - 2

Eu (**period 6**): [Xe] **6**s^2 **4**f^7

Determine the Electron Configuration for Nickel?



1A																7A	8A
1 H	2A											3A	4A	5A	6A	1 H	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg	3B	4B	5B	6B	7B	8B			1B	2B	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
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
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
55 Cs	56 Ba	57 La*	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
87 Fr	88 Ra	89 Ac**	104 Rf	105 Ha	106 Sg	107 Ns	108 Hs	109 Mt	110	111							
	Lanthanide* Series			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
	Actinide** Series			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

Ni is the 8th d-block element in period 4. It has 28 electrons (because Z = 28)

Determine the Electron Configuration for Nickel?

The noble gas preceding Ni is Ar. Ar contains 18 electrons

[Ar]

The 19th and 20th electrons of Ni go into s-orbitals with ***quantum number = period number.***

↳ Ni is in period **4** so the 19th and 20th electrons go into the 4s orbital.

$[Ar]4s^2$

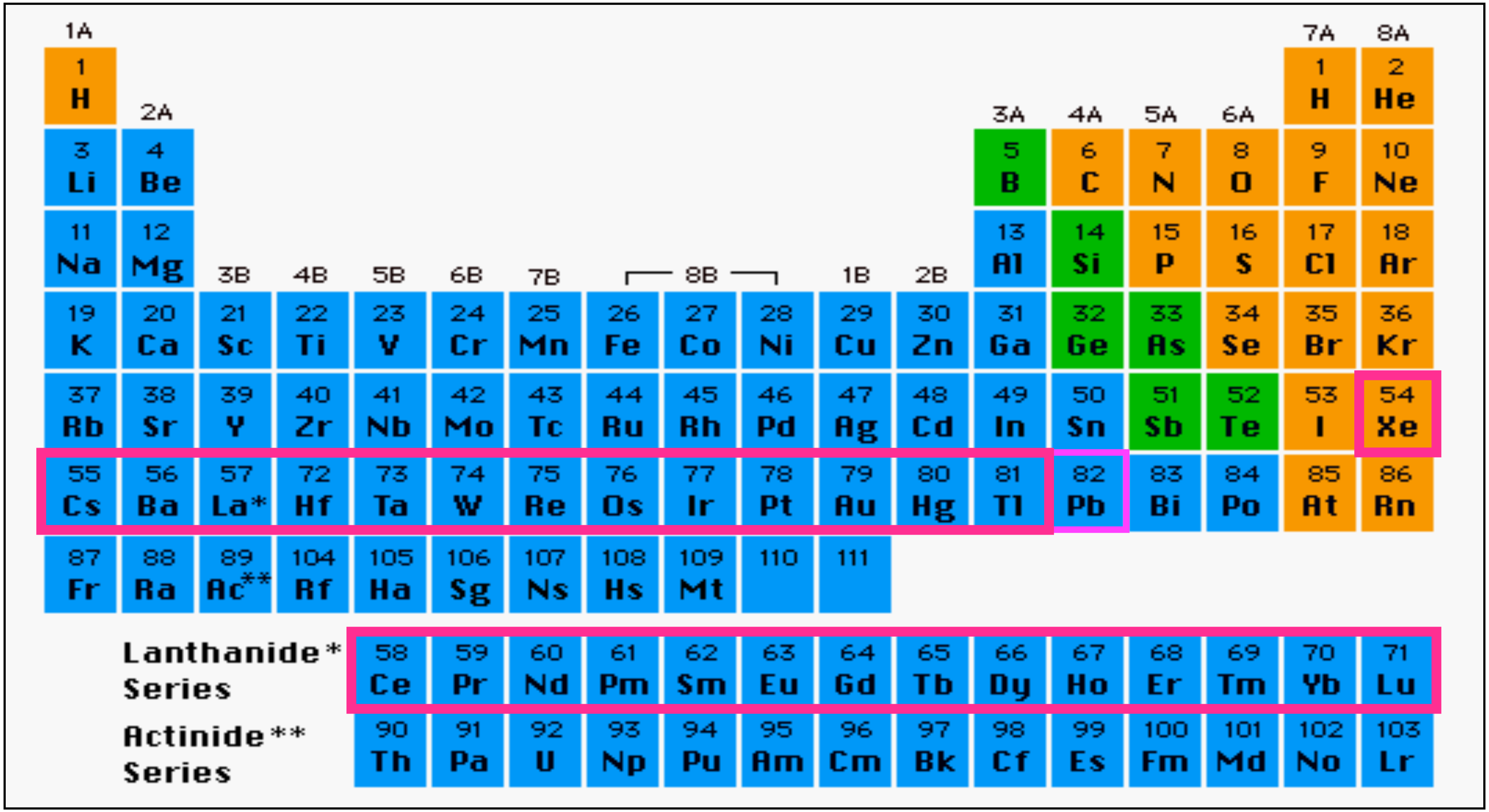
After the s-orbital is full, electrons go into the d-orbitals with ***principle quantum number = period number – 1***

↳ The 21st through 28th electrons go into the **3**d orbital

$[Ar]4s^2 3d^8$

Is this an open or closed shell?

Determine the Electron Configuration for Lead?



1A	2A	3B	4B	5B	6B	7B	8B			1B	2B	3A	4A	5A	6A	7A	8A
1 H																1 H	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
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
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
55 Cs	56 Ba	57 La*	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
87 Fr	88 Ra	89 Ac**	104 Rf	105 Ha	106 Sg	107 Ns	108 Hs	109 Mt	110	111							
Lanthanide* Series				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
Actinide** Series				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

Pb is the 2nd p-block element in period 6. It has 82 electrons (Z = 82)

Electron Configurations of Ions

Ions formed from most elements (not including transition elements) tend to adopt the noble-gas electron configuration.

Cations:

↳ To form cations, electrons are ***removed*** from the ***highest occupied n shell***.

Element	Ion
Na: [Ne] $3s^1$	
Ca: [Ar] $4s^2$	
Al: [Ne] $3s^2 3p^1$	

Anions:

↳ To form anions, electrons are ***added*** to the ***highest partially-filled n shell***.

Element	Ion
F: $1s^2\ 2s^2\ 2p^5$	
O: $1s^2\ 2s^2\ 2p^4$	
N: $1s^2\ 2s^2\ 2p^3$	

F^-, O^{2-}, and N^{3-} have the ***same number of electrons***,

Electron Configurations of Transition Metal Cations

When a cation is formed from an atom of a transition metal, **electrons are almost always removed first from the *s*-orbital** and then from the *d*-orbitals.

Fe: [Ar]$4s^2 3d^6$

Fe^{2+}: [Ar]$4s^0 3d^6$ or [Ar]$3d^6$

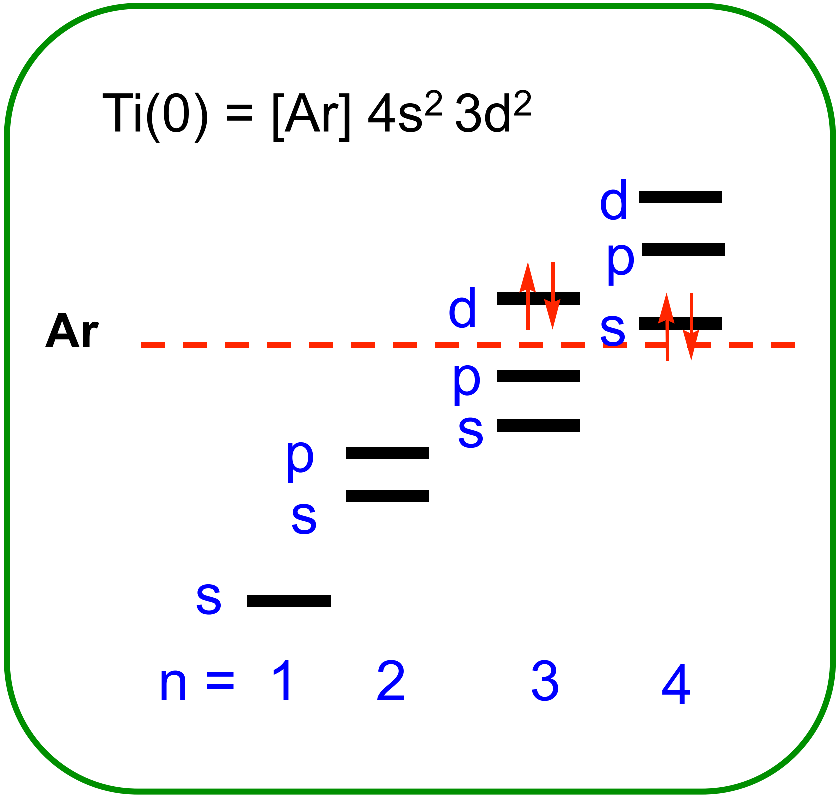
Fe^{3+}: [Ar]$4s^0 3d^5$ or [Ar]$3d^5$

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

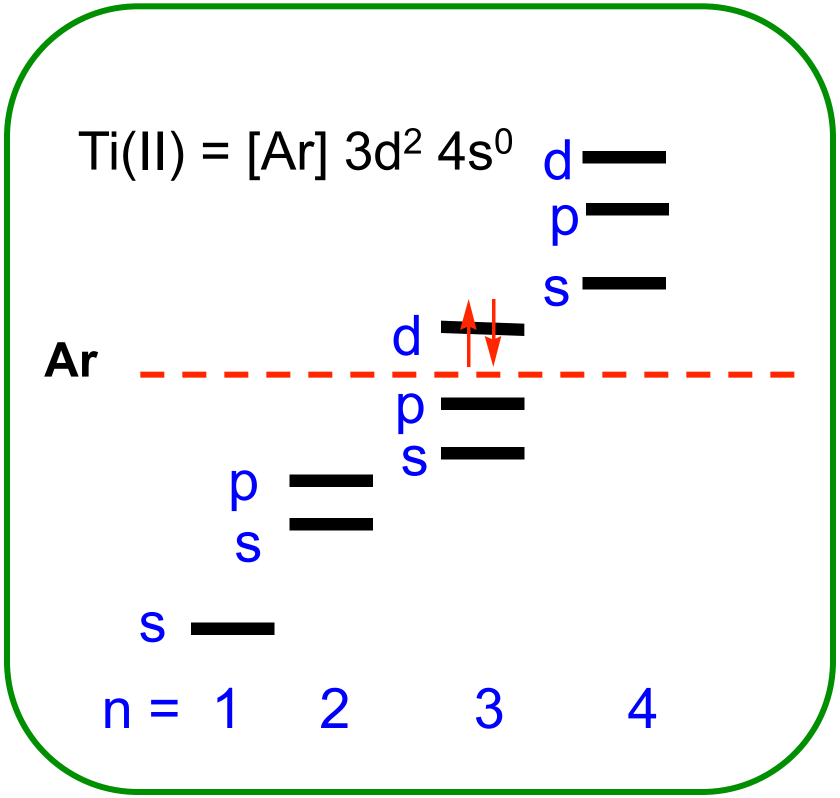
Mn^{2+}: [Ar]$4s^0 3d^5$ or [Ar]$3d^5$

4s electrons are removed *before* 3d electrons are removed.

Transition Metal Atoms and Ions



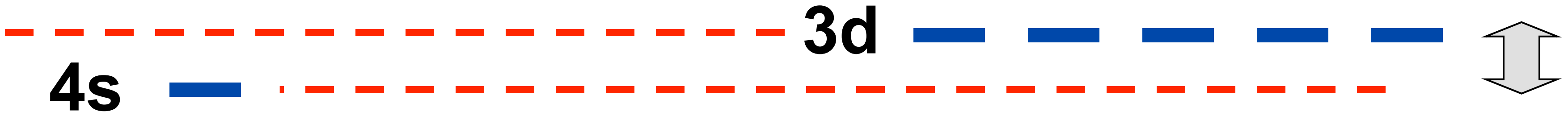
Ti(0) = [Ar] $4s^2\ 3d^2$



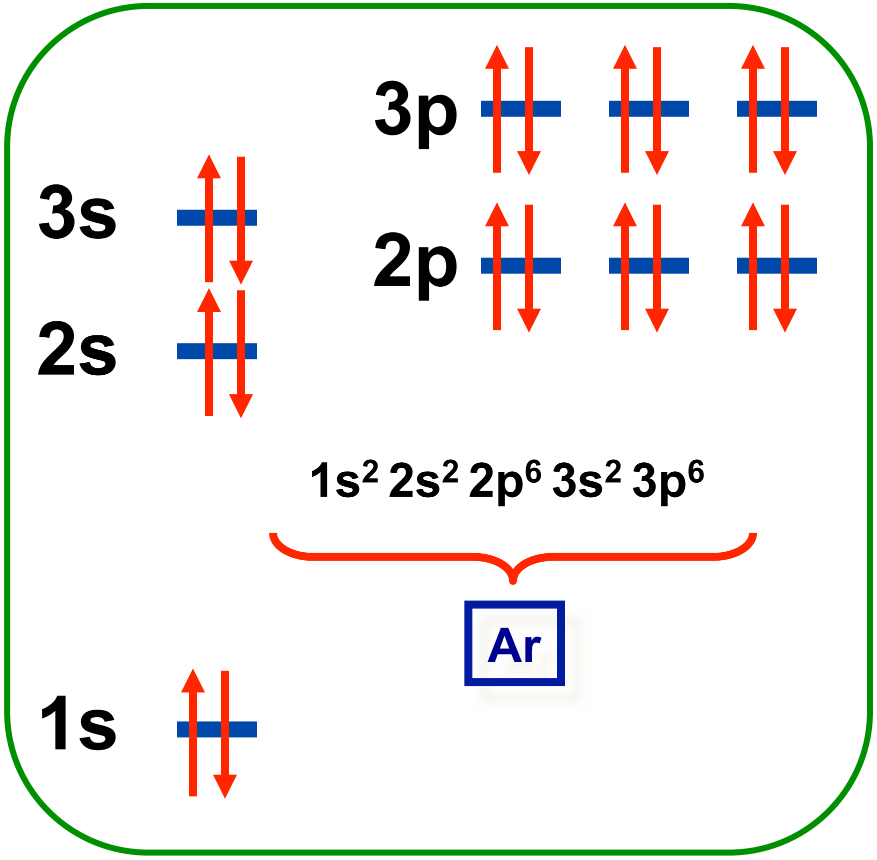
Ti(II) = [Ar] $3d^2\ 4s^0$

With increasing charge levels return to H-like ordering (3d below 4s).

Transition Metal Atoms and Ions



very close, thus . . .



All ½ filled and filled shells are super stable

Cu = [Ar] $4s^1\ 3d^{10}$ 1 UPE

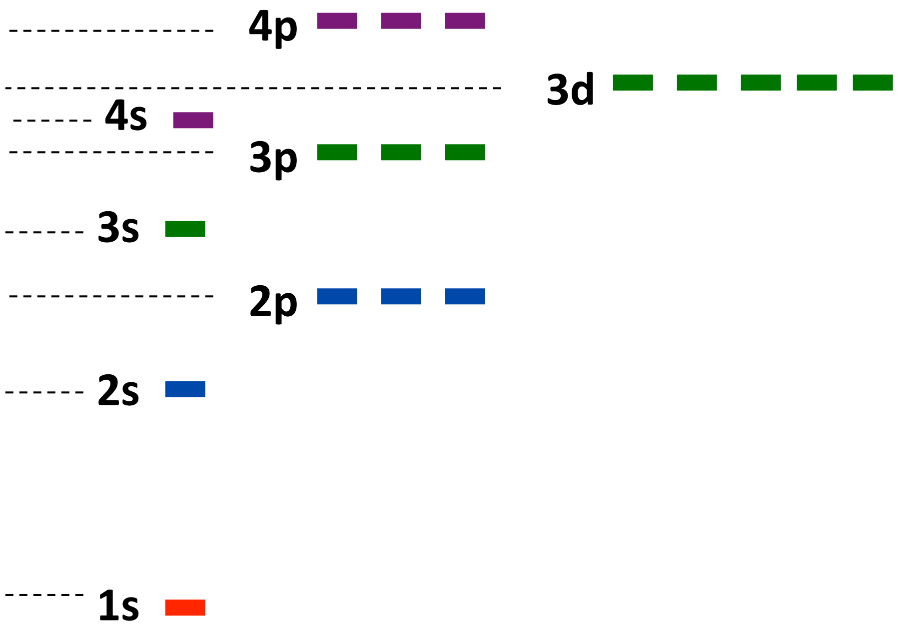
Cr = [Ar] $4s^1\ 3d^5$ 6 UPE

All M^{2+} ions are 3d-only (4s/3d ordering *inverts*)

Fe = [Ar] $4s^2\ 3d^6$ 4 UPE

Fe^{2+} = [Ar] $3d^6$ 4 UPE

Electron Configurations of Atoms & Ions...A Summary

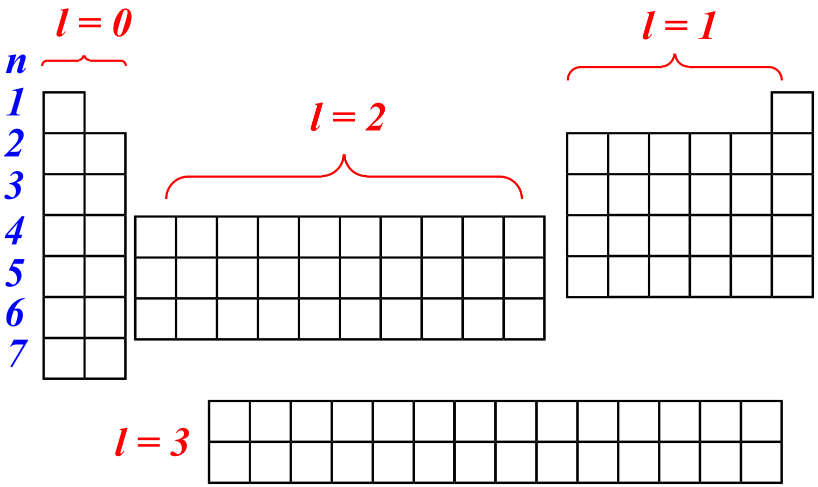


Issues to Understand . . .

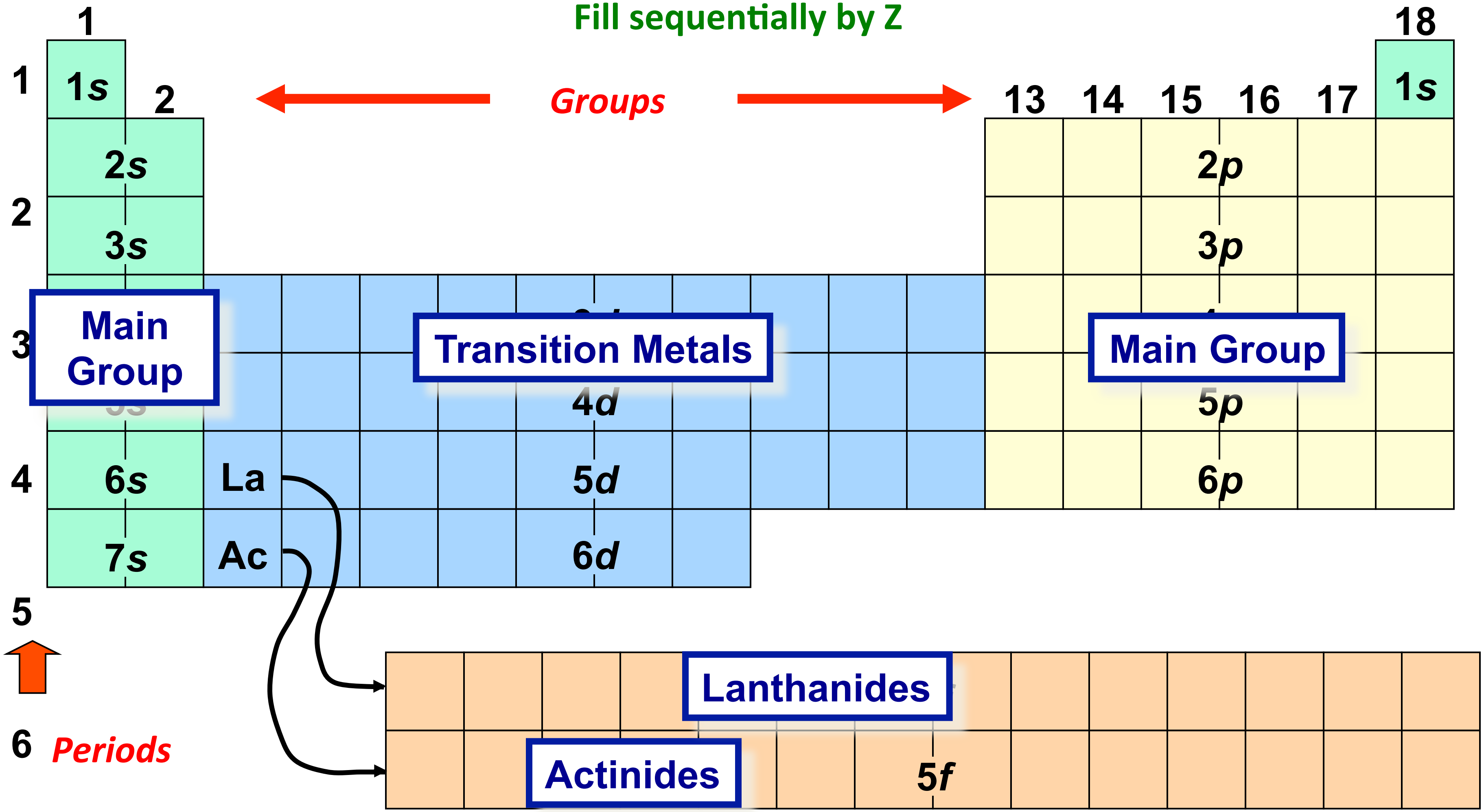
- **Pauli Principle.**
- **Hund's Rule.**
- **Inversion of 4s / 3d levels.**

You should be able to . . .

- Write configuration of any atom or ion.
- Specify valence electrons.
- Specify unpaired electrons.
- Identify isoelectronic pairs.



The Periodic Table



Atomic configuration provides blueprint for properties

Electron Configurations and Periodic Relationships

Many atomic properties are related to the ***electrostatic attraction of electrons to the atomic nucleus***

Periodic Variation in Properties of Atoms:

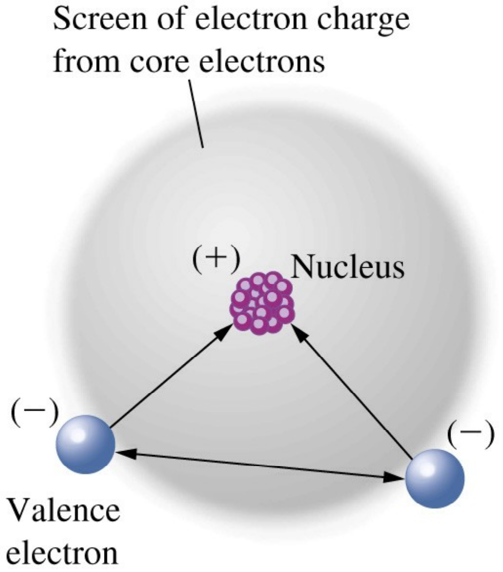
Atomic Radius – attraction between electrons and the nucleus decreases the atomic radius.

Ionization energy – attraction between electrons and the nucleus makes it more difficult to remove an electron.

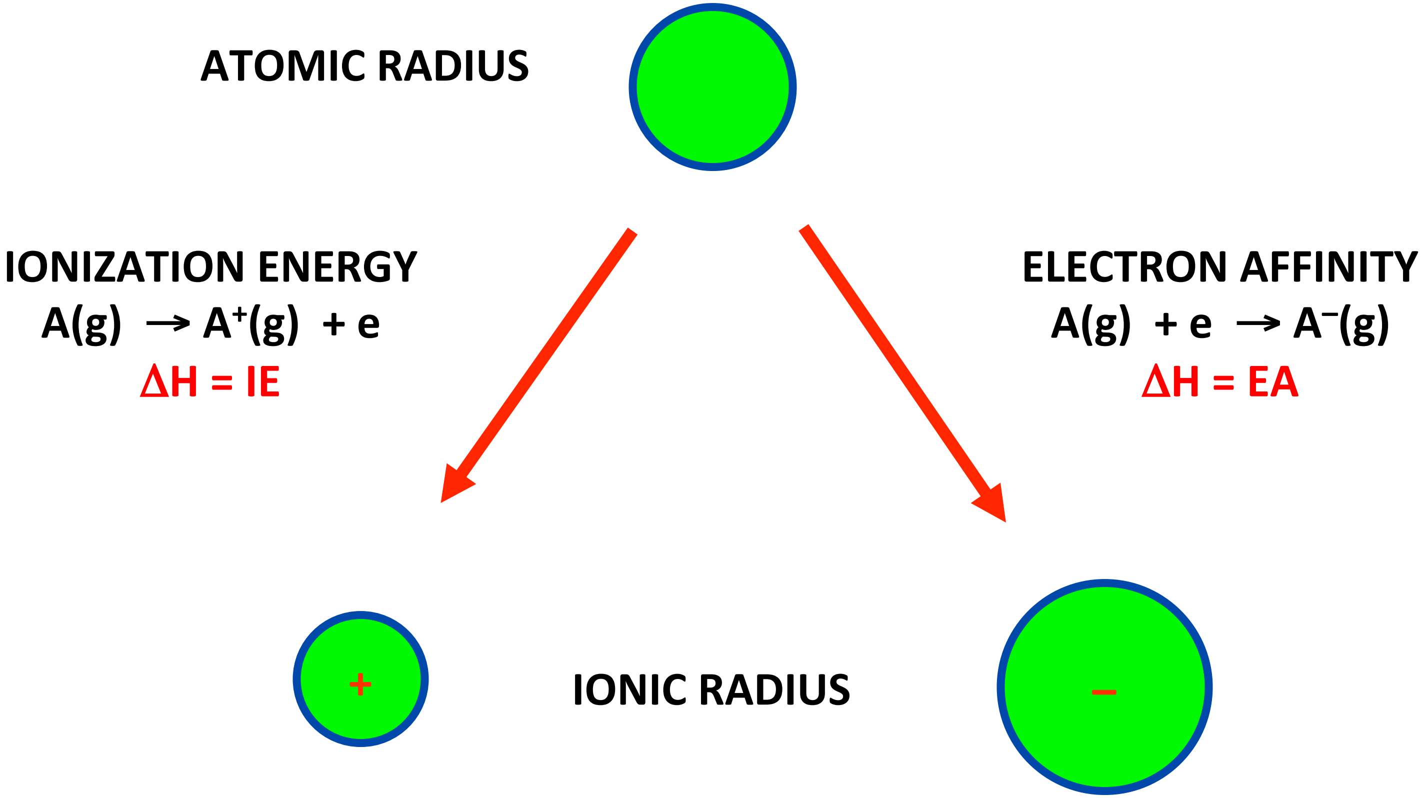
Electron affinity – attraction between electrons and the nucleus makes it easier to add additional electrons to the atom.

Attraction of Electrons to the Nucleus

Electrons in the interior orbitals of an atom ***shield*** outer electrons from the pull of the positively-charged nucleus.



Experimentally Measurable Atomic Properties



ATOMIC RADIUS

IONIZATION ENERGY

$A(g) \rightarrow A^{+}(g) + e$

$\Delta H = IE$

ELECTRON AFFINITY

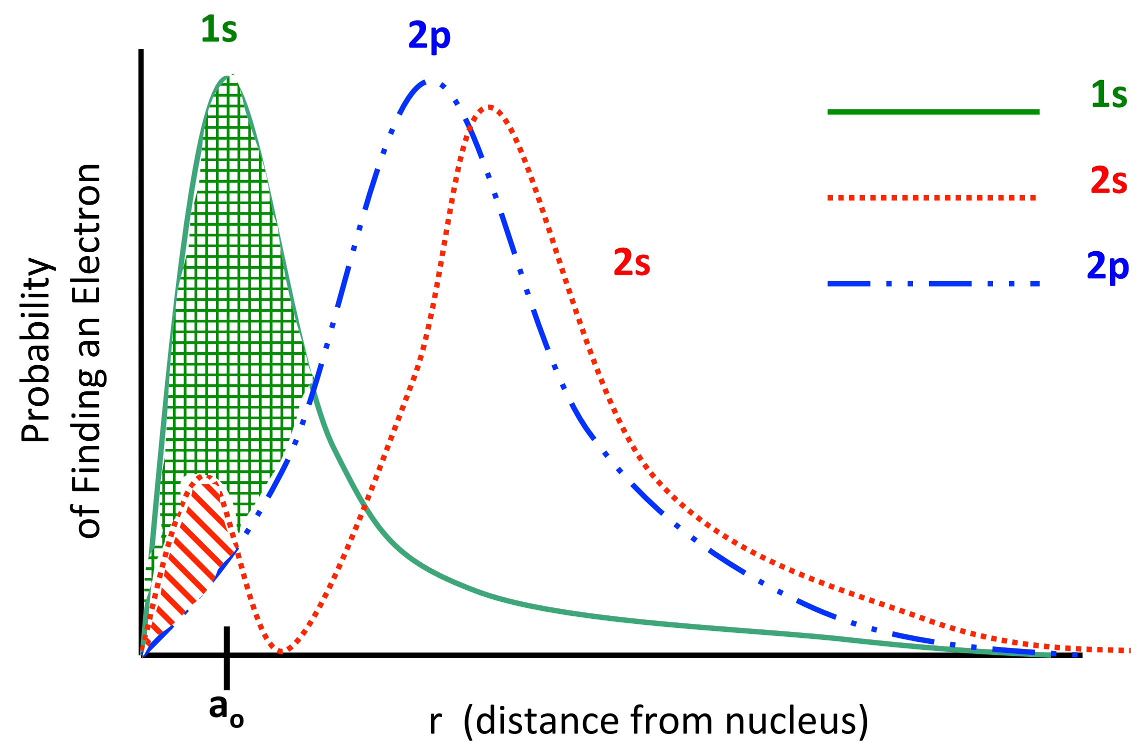
$A(g) + e \rightarrow A^{-}(g)$

$\Delta H = EA$

IONIC RADIUS

These parameters provide the "genetic code" for chemical reactivity of the elements

Orbital Penetration and Electron Shielding



Attraction of Electrons to Nucleus: s > p > d > f

most attracted **least attracted**

Slater's Screening Constant

"**S**" represents the extent to which inner electrons shield the outer electrons from experiencing the pull of the nucleus.

Na: $\underbrace{1s^2\ 2s^2\ 2p^6\ 3s^1}$

Core electrons prevent the 3s electron from experiencing the full charge of the 11 protons in the nucleus.

K: $\underbrace{1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1}$

A larger number of core electrons than for Na. Thus, the **4s** electron in K experiences more shielding (larger S) than the **3s** electron in Na.

Electron Shielding and Z_{eff}

We can quantitatively determine the nuclear charge felt by an electron in a specific orbital using the concept of ***effective nuclear charge***.

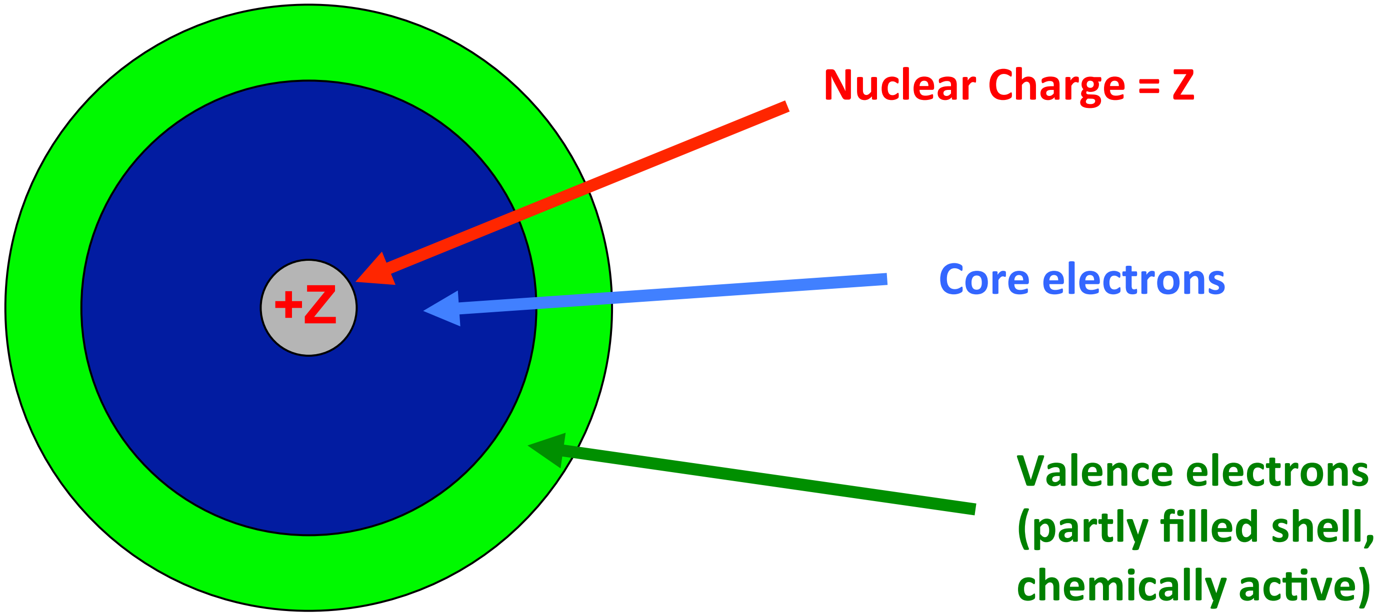
Z_{actual} : the actual charge of the nucleus (# protons)

Effective Nuclear Charge, Z_{eff} : the nuclear charge experienced by a given electron.

$$Z_{eff} = Z_{actual} - S$$

where **S** is "Slater's Screening Constant"

Electron Screening, Z and Z_{eff}



Nuclear Charge = Z

Core electrons

Valence electrons
(partly filled shell,
chemically active)

$\boxed{Z_{eff} = Z - S}$

Z_{eff} is the effective nuclear charge.

Screening (S) reduces Z_{eff}

Quantitative Determination of Z_{eff}: Slater's Rules

1. List orbitals in groups by increasing *n* and group them

   (1s) (2s, 2p) (3s, 3p) (3d) (4s, 4p) (4d) (4f) (5s, 5p) etc.

   ↳ An **ns** and **np** orbital have similar orbital penetration (by this theory) so are grouped together as (**ns**, **np**).

   ↳ An **nd** orbital has less orbital penetration than **ns** and **np**, so is grouped to the right of the (**ns**, **np**) group.

   ↳ An **nf** orbital has even less orbital penetration than **nd**, so is grouped to the right of **nd**

2. Electrons in a group to the right in this list do not shield electrons in a group to the left (because they have less penetration).

Quantitative Determination of Z_{eff}: Slater's Rules

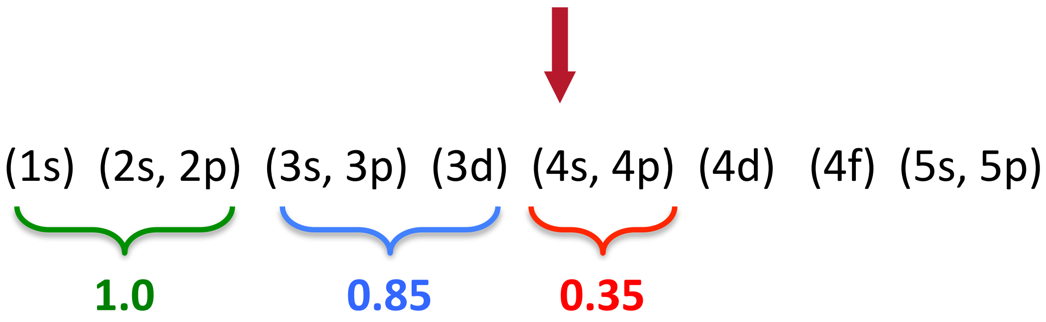
3. An electron's ability to shield other electrons from the nucleus can be quantified using a numerical ***shielding factor, S***.

(a) Calculating S for electrons in **ns** or **np** orbitals:

↳ Each electron in the same **ns** or **np** orbital as the electron of interest contributes **0.35** to the shielding factor (except 1s, which contributes **0.30**)

↳ Electrons in the (**n-1**) level contribute **0.85**.

↳ Electrons in (**n-2**) or lower levels contribute **1.00**.


(1s) (2s, 2p) (3s, 3p) (3d) (4s, 4p) (4d) (4f) (5s, 5p)

1.0 **0.85** **0.35**

Quantitative Determination of Z_{eff}: Slater's Rules

3. An electron's ability to shield other electrons from the nucleus can be quantified using a numerical ***shielding factor, S***.

(b) Calculating S for electrons in **nd** or **nf** orbitals:

↳ Electrons in the same **nd** or **nf** level contribute **0.35** to the shielding factor.

↳ Electrons in orbital groupings to the left of the one in question contribute **1.00**.

$$\underbrace{(1s)\ (2s, 2p)\ (3s, 3p)\ (3d)\ (4s, 4p)\ (4d)}_{1.0}\ \underbrace{\overset{\big\downarrow}{(4f)}}_{0.35}\ (5s, 5p)$$

4. The calculated S is subtracted from the true nuclear charge, Z_{actual}, to determine the effective nuclear charge, Z_{eff}.

$$\boxed{Z_{eff} = Z_{actual} - S}$$

Example Calculation of Z_{eff}

Calculate Z_{eff} for a 3d electron in Titanium:

$$Z_{eff} = Z_{actual} - S$$

1) Determine the electron configuration of Ti:

$$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^2$$

2) Determine orbital groupings:

$$\boxed{(1s^2)\ \ (2s^2, 2p^6)\ \ (3s^2, 3p^6)}\ \boxed{(3d^2)}\ \xcancel{(4s^2, 4p^0)}$$

3) Rule 2: Electrons in orbitals to the right don't shield electrons in orbitals to the left
→ the 2 electrons in 4s don't contribute to shielding

4) Rule 3b: Electrons in the same **nd** orbital contribute 0.35. All other electrons contribute 1.00.

$$S = (0.35 \times 1) + (1.00 \times 18) = 18.35$$

5) The calculated S is subtracted from the true nuclear charge, Z_{actual}, to determine the effective nuclear charge, Z_{eff}.

↳ Z_{actual} = 22 because there are 22 protons (atomic number)

$$\begin{aligned} Z_{eff} &= 22 - 18.35 \\ &= 3.65 \end{aligned}$$

The actual charge of the nucleus for Titanium is 22.
The nuclear charge felt by an electron in the 3d orbital is 3.65

Exercise

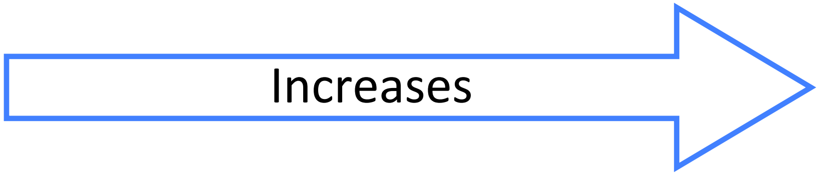
Calculate Z_{eff} for the following:

1) An electron in the 2p orbital of boron (Z = 5)
2) And electron in the 2p orbital of oxygen (Z = 8)

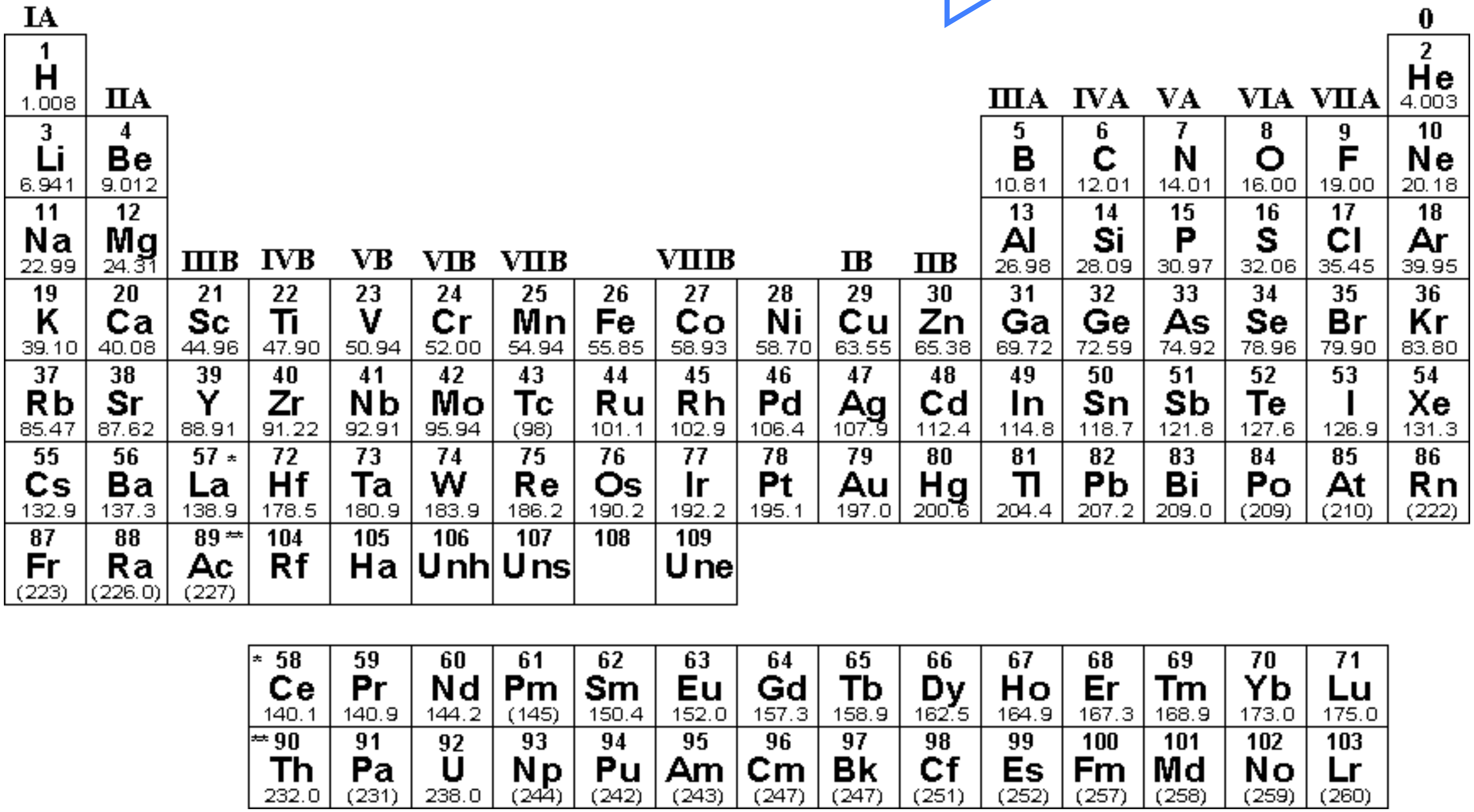
From this, what would you conclude about the trend in Z_{eff} as you move from left to right across a period?

Effective Nuclear Charge

General Trend


Increases

Due to increasing
protons



IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB			IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
1 **H** 1.008																	2 **He** 4.003
3 **Li** 6.941	4 **Be** 9.012											5 **B** 10.81	6 **C** 12.01	7 **N** 14.01	8 **O** 16.00	9 **F** 19.00	10 **Ne** 20.18
11 **Na** 22.99	12 **Mg** 24.31											13 **Al** 26.98	14 **Si** 28.09	15 **P** 30.97	16 **S** 32.06	17 **Cl** 35.45	18 **Ar** 39.95
19 **K** 39.10	20 **Ca** 40.08	21 **Sc** 44.96	22 **Ti** 47.90	23 **V** 50.94	24 **Cr** 52.00	25 **Mn** 54.94	26 **Fe** 55.85	27 **Co** 58.93	28 **Ni** 58.70	29 **Cu** 63.55	30 **Zn** 65.38	31 **Ga** 69.72	32 **Ge** 72.59	33 **As** 74.92	34 **Se** 78.96	35 **Br** 79.90	36 **Kr** 83.80
37 **Rb** 85.47	38 **Sr** 87.62	39 **Y** 88.91	40 **Zr** 91.22	41 **Nb** 92.91	42 **Mo** 95.94	43 **Tc** (98)	44 **Ru** 101.1	45 **Rh** 102.9	46 **Pd** 106.4	47 **Ag** 107.9	48 **Cd** 112.4	49 **In** 114.8	50 **Sn** 118.7	51 **Sb** 121.8	52 **Te** 127.6	53 **I** 126.9	54 **Xe** 131.3
55 **Cs** 132.9	56 **Ba** 137.3	57 * **La** 138.9	72 **Hf** 178.5	73 **Ta** 180.9	74 **W** 183.9	75 **Re** 186.2	76 **Os** 190.2	77 **Ir** 192.2	78 **Pt** 195.1	79 **Au** 197.0	80 **Hg** 200.6	81 **Tl** 204.4	82 **Pb** 207.2	83 **Bi** 209.0	84 **Po** (209)	85 **At** (210)	86 **Rn** (222)
87 **Fr** (223)	88 **Ra** (226.0)	89 ** **Ac** (227)	104 **Rf**	105 **Ha**	106 **Unh**	107 **Uns**	108	109 **Une**									

* 58 **Ce** 140.1	59 **Pr** 140.9	60 **Nd** 144.2	61 **Pm** (145)	62 **Sm** 150.4	63 **Eu** 152.0	64 **Gd** 157.3	65 **Tb** 158.9	66 **Dy** 162.5	67 **Ho** 164.9	68 **Er** 167.3	69 **Tm** 168.9	70 **Yb** 173.0	71 **Lu** 175.0
** 90 **Th** 232.0	91 **Pa** (231)	92 **U** 238.0	93 **Np** (244)	94 **Pu** (242)	95 **Am** (243)	96 **Cm** (247)	97 **Bk** (247)	98 **Cf** (251)	99 **Es** (252)	100 **Fm** (257)	101 **Md** (258)	102 **No** (259)	103 **Lr** (260)

Slater Rules: A Shortcoming

Orbitals are listed in groups:

(1s) (2s, 2p) (3s, 3p) (3d) (4s, 4p) (4d) (4f) (5s, 5p)

This grouping implies that ns and np electrons experience the same shielding. They don't!

The model still works quite well anyway.

Electron Configurations and Periodic Relationships

Many atomic properties are related to the ***electrostatic attraction of electrons to the atomic nucleus***

Periodic Variation in Properties of Atoms:

Atomic Radius – attraction between electrons and the nucleus decreases the atomic radius.

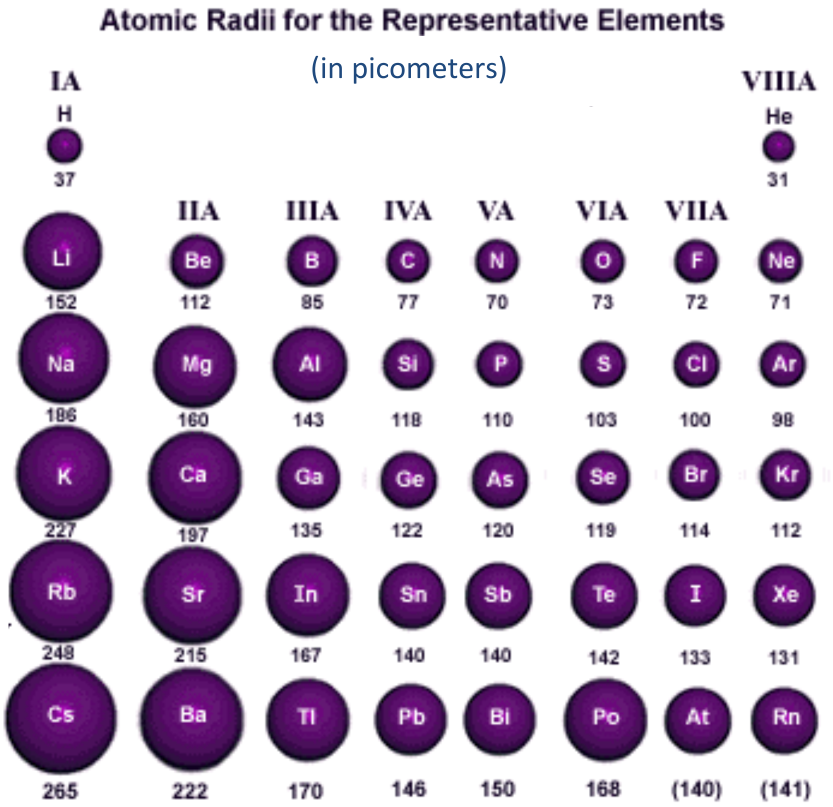
Ionization energy – attraction between electrons and the nucleus makes it more difficult to remove an electron.

Electron affinity – attraction between electrons and the nucleus makes it easier to add additional electrons to the atom.

Atomic Radius

Atomic radius is determined by the size of the **outermost** orbital containing electrons.

Attractions of the outer electrons to the nucleus (i.e. higher Z_{eff}) result in   in the orbital size



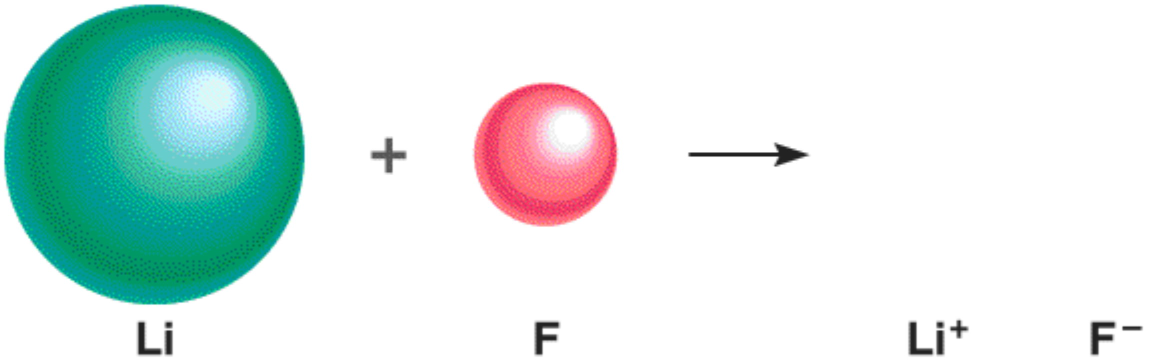
Atomic Radii for the Representative Elements

(in picometers)

IA	IIA	IIIA	IVA	VA	VIA	VIIA	VIIIA
H 37							He 31
Li 152	Be 112	B 85	C 77	N 70	O 73	F 72	Ne 71
Na 186	Mg 160	Al 143	Si 118	P 110	S 103	Cl 100	Ar 98
K 227	Ca 197	Ga 135	Ge 122	As 120	Se 119	Br 114	Kr 112
Rb 248	Sr 215	In 167	Sn 140	Sb 140	Te 142	I 133	Xe 131
Cs 265	Ba 222	Tl 170	Pb 146	Bi 150	Po 168	At (140)	Rn (141)

- ➥ Atomic radius DECREASES across a period as Z_{eff} INCREASES
- ➥ Atomic radius INCREASES down a group as principle quantum number, n, increases.

Ionic Radius

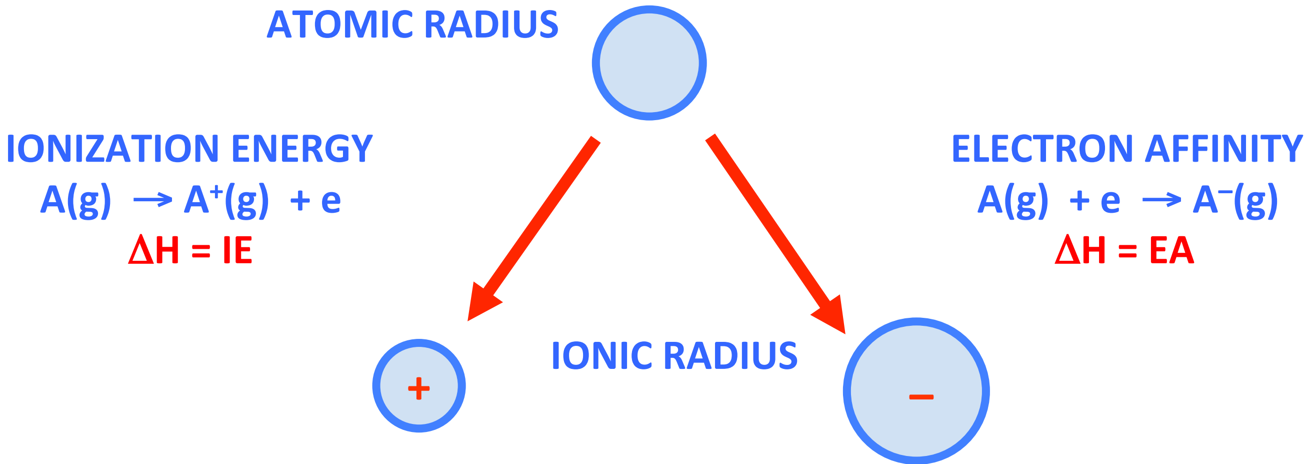


Cation is always **smaller** than the atom from which it is formed.

Anion is always **larger** than the atom from which it is formed.

Why?

Atomic vs Ionic Radii



ATOMIC RADIUS

IONIZATION ENERGY

$A(g) \rightarrow A^{+}(g) + e$

$\Delta H = IE$

ELECTRON AFFINITY

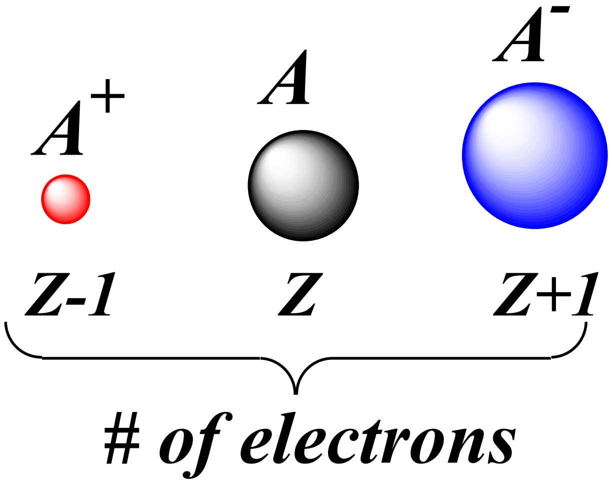
$A(g) + e \rightarrow A^{-}(g)$

$\Delta H = EA$

IONIC RADIUS

Ionic Size and Trends in Ionic Radii

Size decreases as Z_{eff} increases, hence . . .



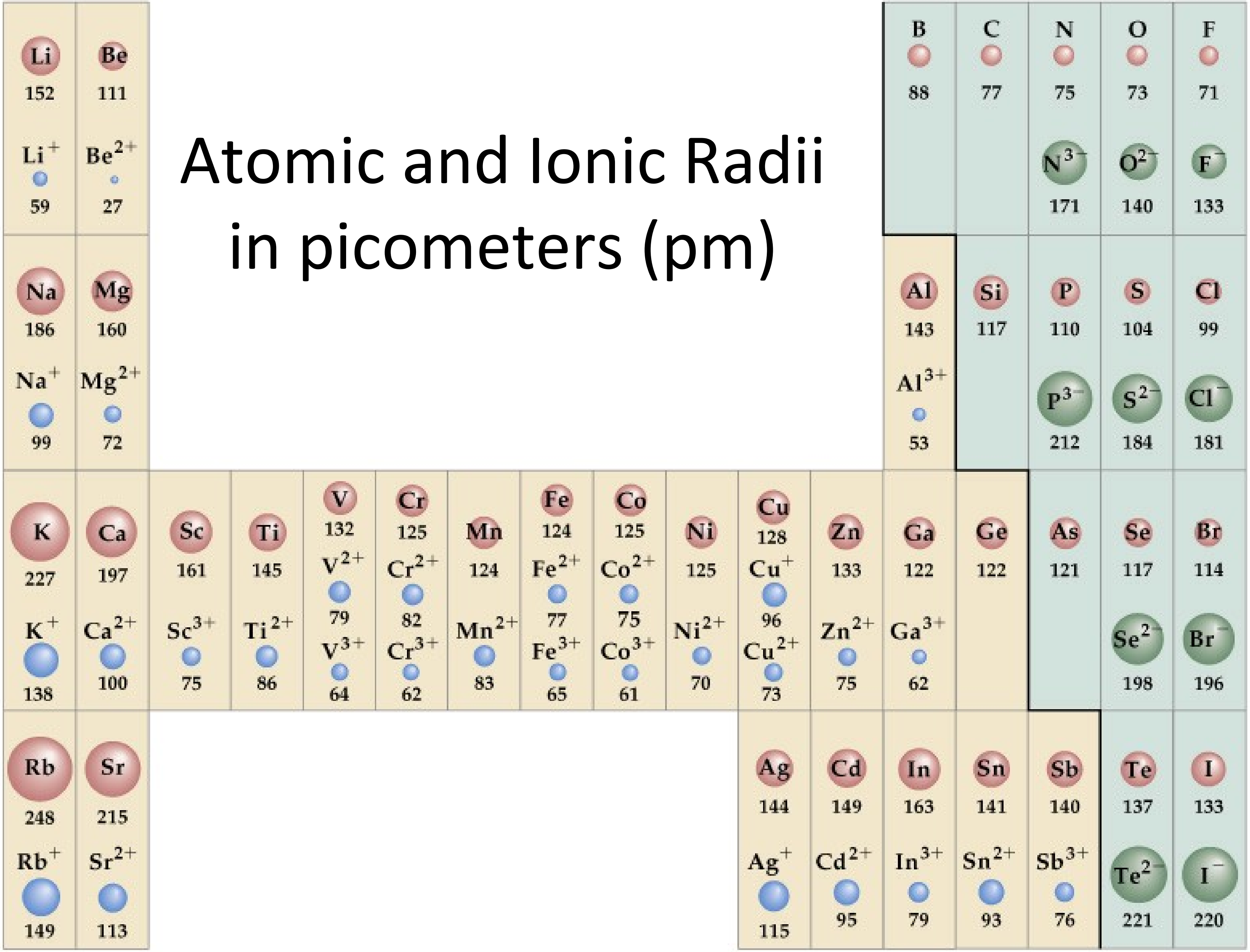
Within an *isoelectronic* series . . .

$O^{2-} > F^{-} > [\mathrm{Ne}] > Na^{+} > Mg^{2+} > Al^{3+}$

Within a Periodic Group

$Cl^{-} < Br^{-} < I^{-}$

Atomic and Ionic Radii in picometers (pm)



Li 152	Be 111											B 88	C 77	N 75	O 73	F 71
Li^+ 59	Be^{2+} 27													N^{3-} 171	O^{2-} 140	F^- 133
Na 186	Mg 160											Al 143	Si 117	P 110	S 104	Cl 99
Na^+ 99	Mg^{2+} 72											Al^{3+} 53		P^{3-} 212	S^{2-} 184	Cl^- 181
K 227	Ca 197	Sc 161	Ti 145	V 132	Cr 125	Mn 124	Fe 124	Co 125	Ni 125	Cu 128	Zn 133	Ga 122	Ge 122	As 121	Se 117	Br 114
K^+ 138	Ca^{2+} 100	Sc^{3+} 75	Ti^{2+} 86	V^{2+} 79 V^{3+} 64	Cr^{2+} 82 Cr^{3+} 62	Mn^{2+} 83	Fe^{2+} 77 Fe^{3+} 65	Co^{2+} 75 Co^{3+} 61	Ni^{2+} 70	Cu^+ 96 Cu^{2+} 73	Zn^{2+} 75	Ga^{3+} 62			Se^{2-} 198	Br^- 196
Rb 248	Sr 215									Ag 144	Cd 149	In 163	Sn 141	Sb 140	Te 137	I 133
Rb^+ 149	Sr^{2+} 113									Ag^+ 115	Cd^{2+} 95	In^{3+} 79	Sn^{2+} 93	Sb^{3+} 76	Te^{2-} 221	I^- 220

Exercise

Arrange the atoms and ions in each series below in order from smallest to largest radius:

a) Ca^{2+}, S^{2-}, K^{+}, Cl^{-}, Ar

b) Sr, Mg, Ca, Be, Ba, Ra

Ionization Energy / Ionization Potential

The energy needed to remove an electron from the ***outermost occupied orbital*** of a gas-phase atom (measured experimentally):

$$X(g) \rightarrow X^{+}(g) + e^{-}$$

UNITS: Ionization energy (or ionization potential) is given in
kJ/mol, kcal/mol, or eV
(1 eV = 1.602 x 10^{-19} J)

Ionization is ***always endothermic***: energy must be added in order to remove an electron.

Atomic Radii and First Ionization Energies of the Alkali Metal (Group 1) Elements

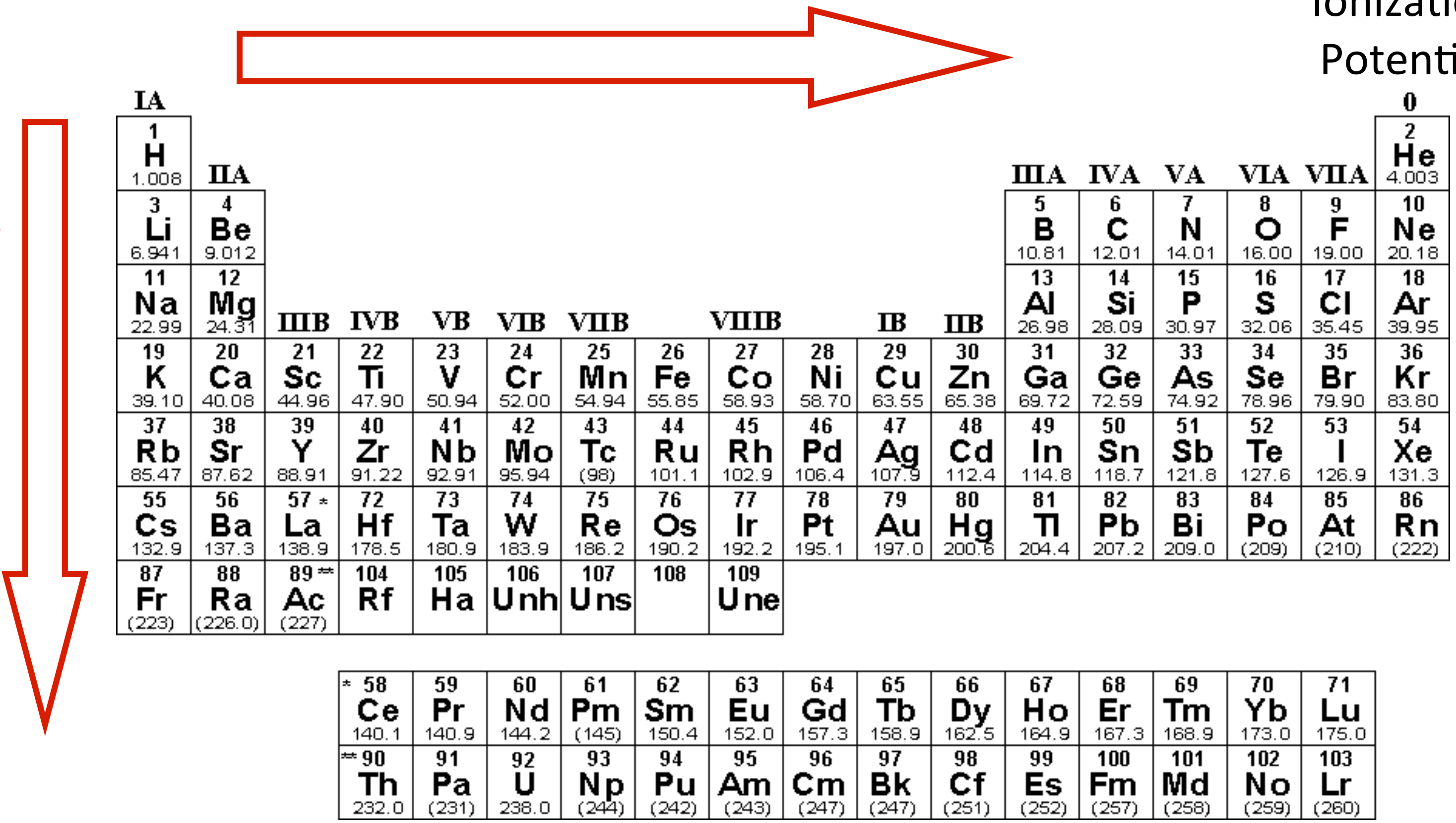
	Atomic Radius, pm	Ionization Energy (I_1), kJ/mol
Li	152	520.2
Na	186	495.8
K	227	418.8
Rb	248	403.0
Cs	265	375.7

The farther an electron is from the nucleus, the easier it is to remove.

larger atomic radius

lower ionization energy

Ionization Energy



increases (due to increasing Z_{eff})

Higher
Ionization
Potential

decreases (due
to increasing
atomic radius)

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB			IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
1 H 1.008																	2 He 4.003
3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
11 Na 22.99	12 Mg 24.31											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.06	17 Cl 35.45	18 Ar 39.95
19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.90	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.70	29 Cu 63.55	30 Zn 65.38	31 Ga 69.72	32 Ge 72.59	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98)	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3
55 Cs 132.9	56 Ba 137.3	57 * La 138.9	72 Hf 178.5	73 Ta 180.9	74 W 183.9	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.6	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226.0)	89 ** Ac (227)	104 Rf	105 Ha	106 Unh	107 Uns	108	109 Une									

* 58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm (145)	62 Sm 150.4	63 Eu 152.0	64 Gd 157.3	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0	71 Lu 175.0
** 90 Th 232.0	91 Pa (231)	92 U 238.0	93 Np (244)	94 Pu (242)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (260)

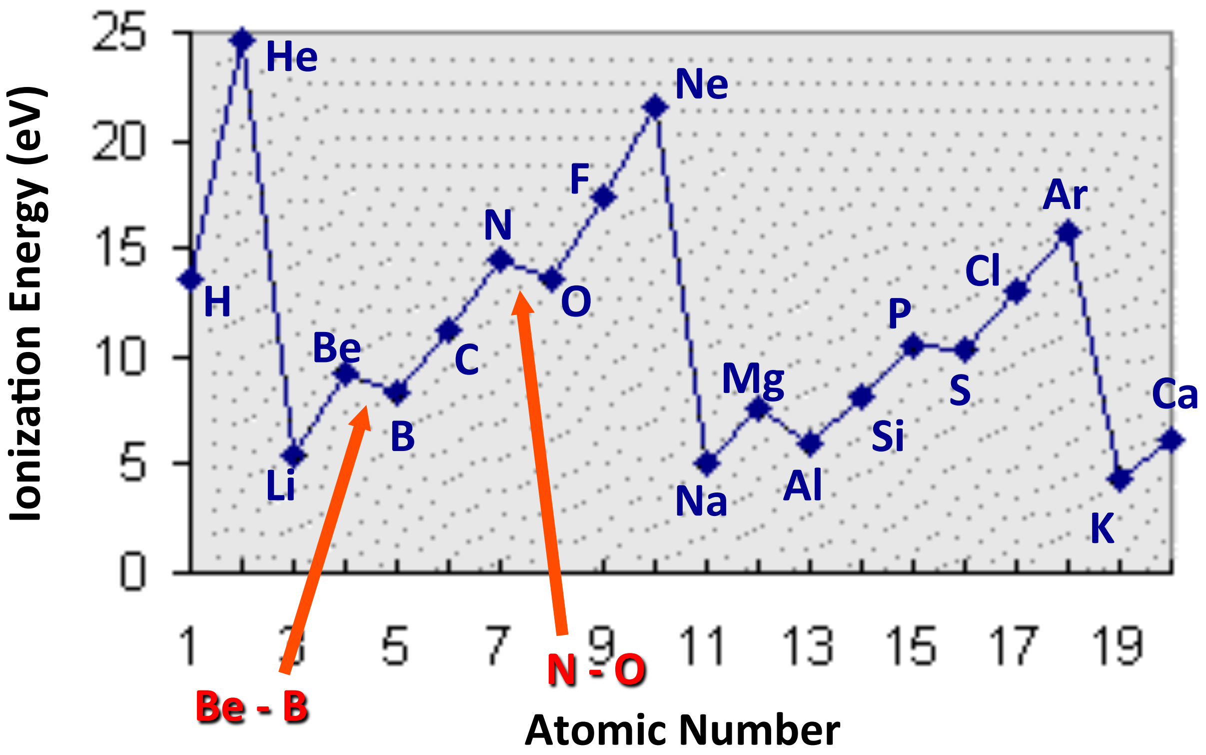
The ***more*** an electron is attracted to the nucleus (higher Z_{eff}), the ***harder*** it will be to remove the electron. This results in a ***higher ionization energy.***

Ionization Energy Trend

In every period, there are two exceptions to the ionization energy trend:

- ➥ Group 2 to Group 13
- ➥ Group 15 to Group 16

Ionization Energies of the First Twenty Elements



Exceptions to Ionization Energy Trends

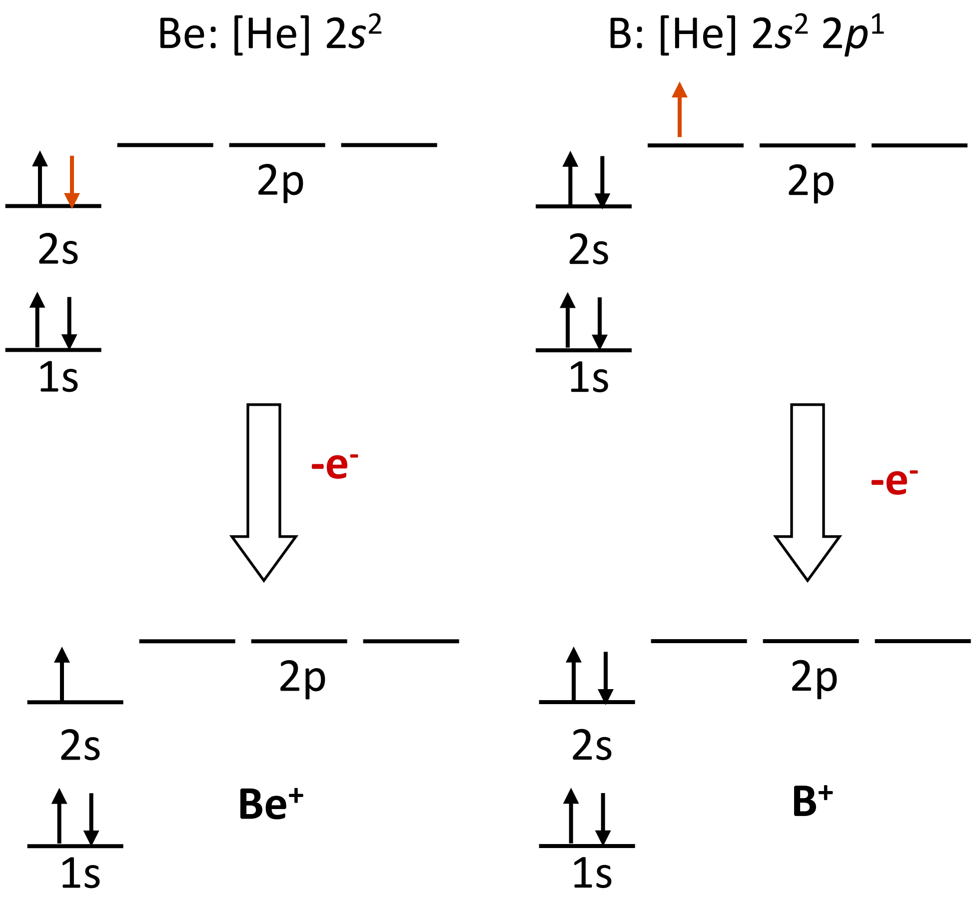
The first ionization energy of boron is smaller than beryllium.

WHY?

It is well illustrated by orbital energy diagrams (to the right):

↳ The 2p orbital is slightly higher in energy than the 2s orbital

↳ less energy is required to remove an electron from a higher energy orbital



Be: [He] $2s^2$

B: [He] $2s^2\ 2p^1$

Higher ionization energy

Lower ionization energy

Exceptions to Ionization Energy Trends

The first ionization energy of oxygen is smaller than nitrogen.

WHY?

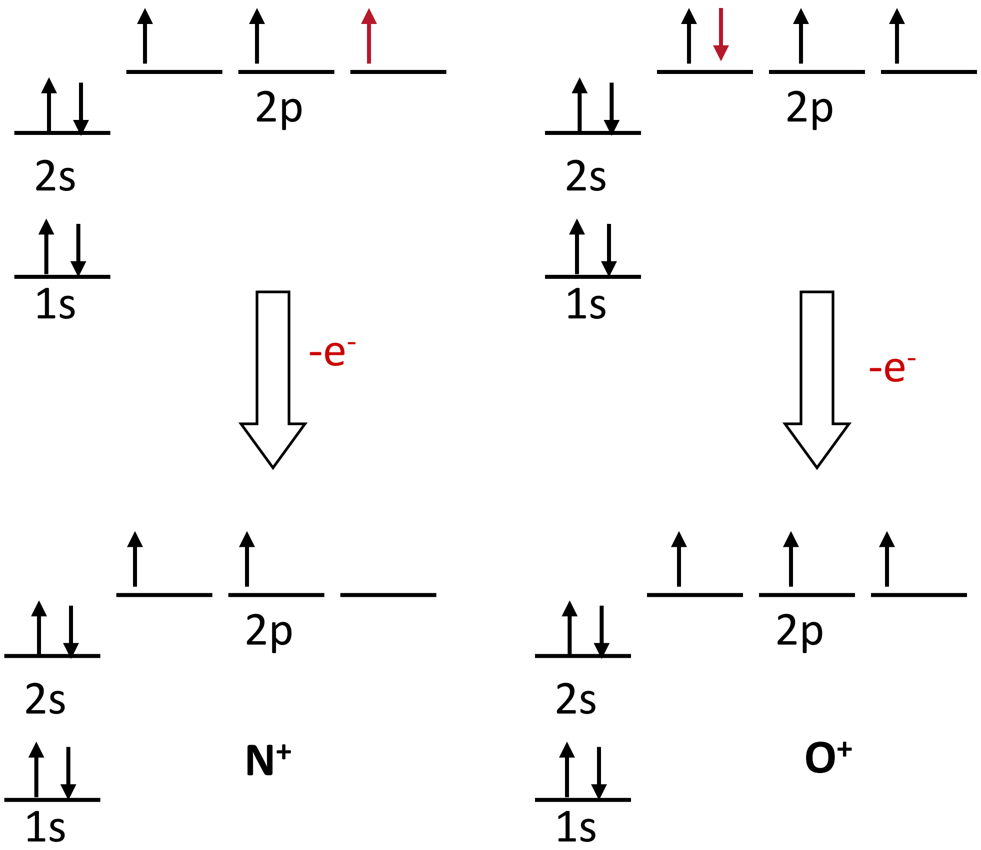
↳ Pairing electrons is unfavorable (e^- - e^- repulsion)

↳ This repulsion destabilizes the O 2p orbital containing 2 e^-

↳ It is easier to remove one of these paired electrons

N: [He] $2s^2\ 2p^3$

O: [He] $2s^2\ 2p^4$

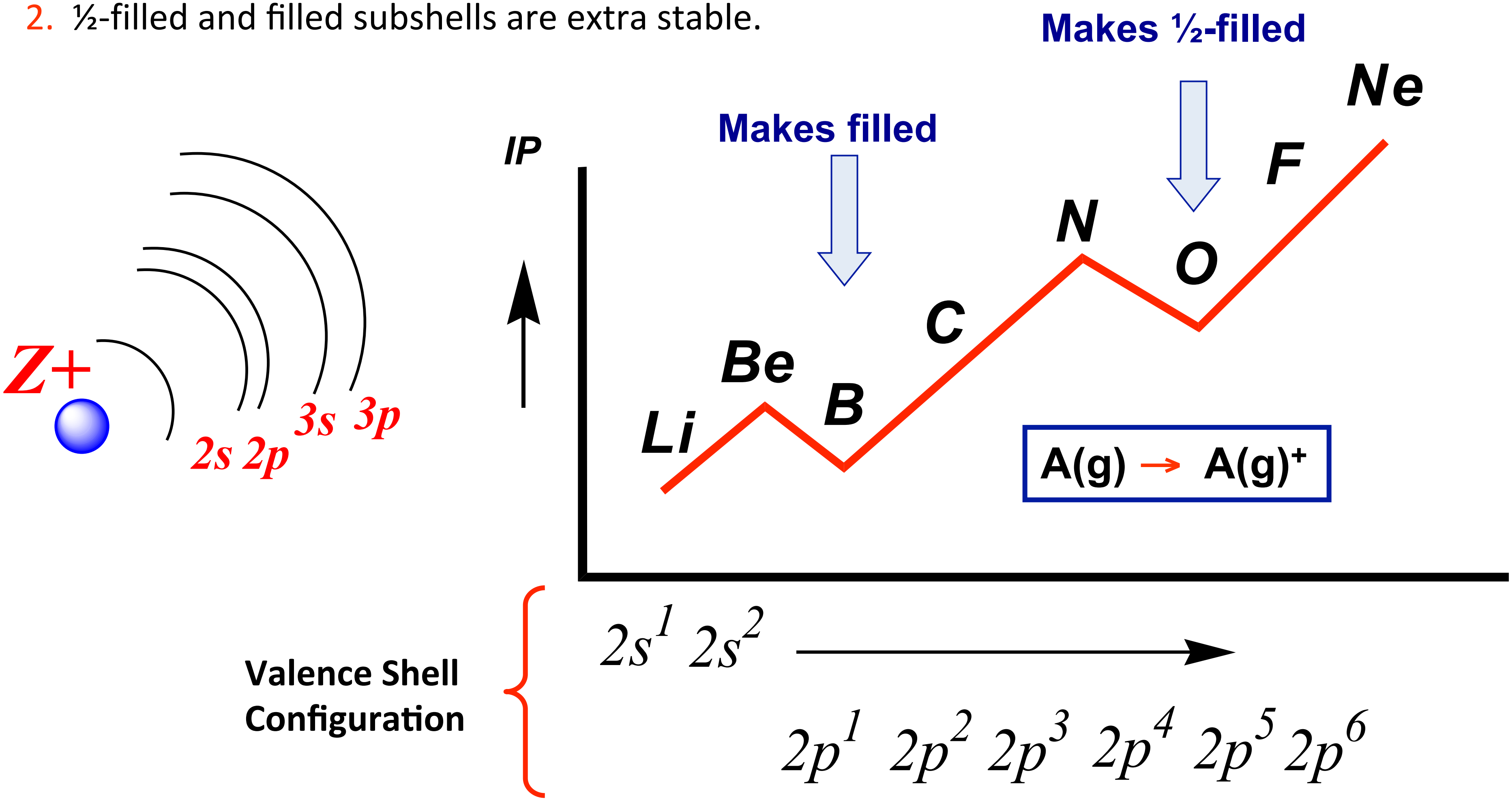


Higher ionization energy

Lower ionization energy

Ionization Energy Trends

1. Z_{eff} (and hence IP) increases across any Period.
2. ½-filled and filled subshells are extra stable.

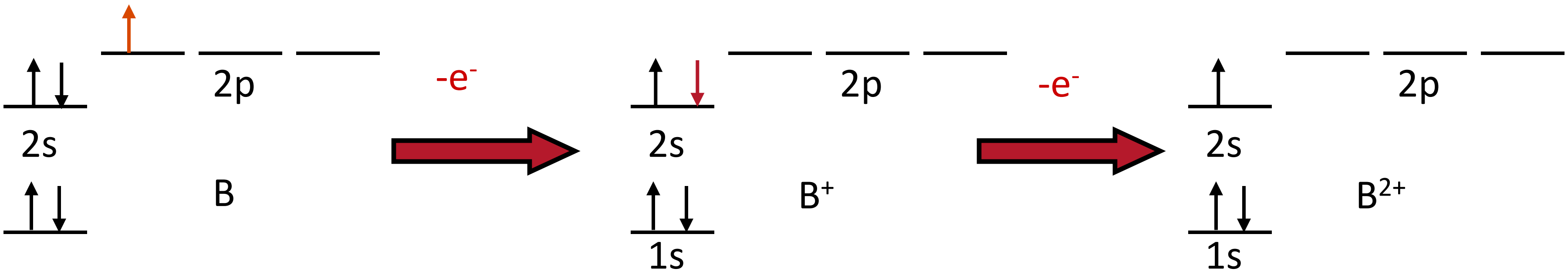


Second Ionization Energy

$$X^+ (g) \rightarrow X^{2+} (g) + e^-$$

In general, the 2nd ionization energy for any atom is **much higher** than the 1st ionization energy:

1. The Z_{eff} is higher for the valence e^- in X^+ than for X
   - ↳ one electron has been removed so the remaining electrons feel a greater attraction to the nucleus.
   - ↳ more energy is needed to liberate another electron.
2. The orbital from which the 2nd electron is removed may (in some cases) be at a lower energy (more stable).



Exercise

Looking at phosphorus and sulfur:

1) Which has a higher Z_{eff}?
2) Based on the Z_{eff} alone, which would you expect to have a higher ionization energy?
3) In reality, which has a higher ionization energy? Why? Use an orbital energy level diagram to support your argument.

Electron Affinity

The energy change upon ***adding an electron*** to the outer-most orbital of an atom in the gaseous state.

$F\ (g) + e^- \rightarrow F^-\ (g)$ $\Delta H = -328$ kJ/mol **(EXOTHERMIC!)**

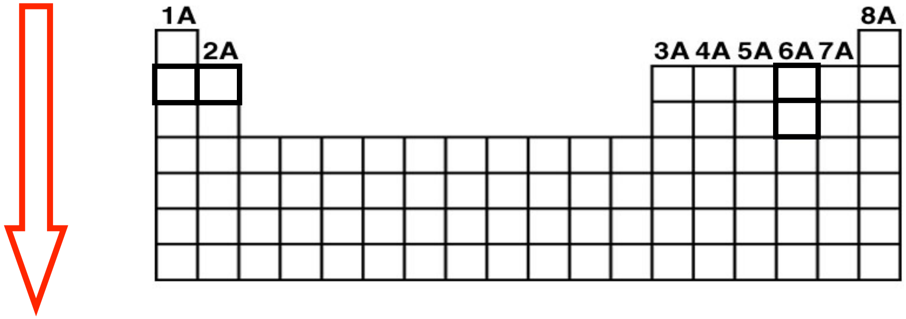
Electron Affinity of F is -328 kJ/mol

Adding an electron is usually energetically FAVORABLE!

Adding an electron becomes ***energetically favorable moving down a group*** because electrons are farther from the nucleus.

Thus, ***electron affinity*** becomes ***negative*** moving down the group.

Electron affinity
becomes less
negative



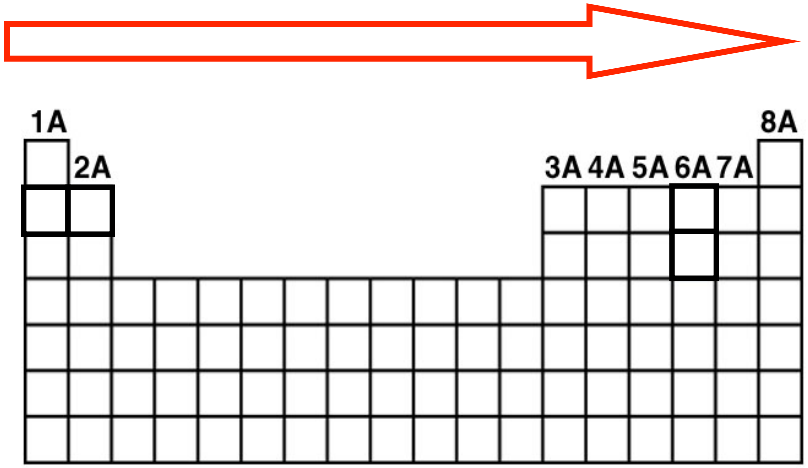
Electron Affinity

Adding an electron becomes ***more energetically favorable moving across a period.***

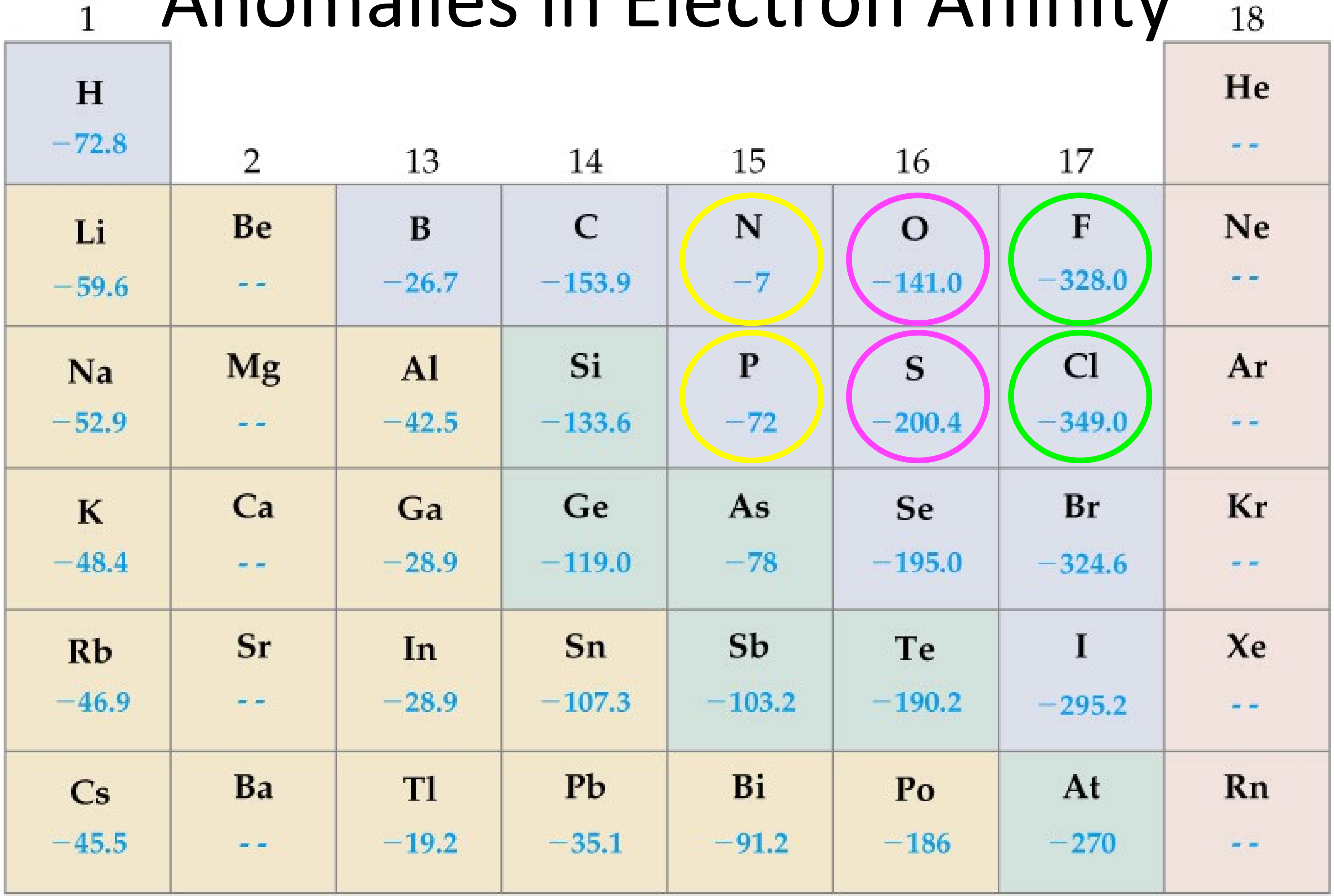
↳ Z_{eff} increases

↳ Attraction of added electrons to the nucleus increases

Thus, ***electron affinity*** becomes ***more negative*** moving across the group.



Anomalies in Electron Affinity



1	2	13	14	15	16	17	18
H −72.8							He - -
Li −59.6	Be - -	B −26.7	C −153.9	N −7	O −141.0	F −328.0	Ne - -
Na −52.9	Mg - -	Al −42.5	Si −133.6	P −72	S −200.4	Cl −349.0	Ar - -
K −48.4	Ca - -	Ga −28.9	Ge −119.0	As −78	Se −195.0	Br −324.6	Kr - -
Rb −46.9	Sr - -	In −28.9	Sn −107.3	Sb −103.2	Te −190.2	I −295.2	Xe - -
Cs −45.5	Ba - -	Tl −19.2	Pb −35.1	Bi −91.2	Po −186	At −270	Rn - -

Anomalies in Electron Affinity

1. Noble gases and alkaline earth metals have ***positive*** electron affinities (adding an electron is unfavorable).

2. For each period, adding an electron to group 15 is ***less*** favourable than adding an electron to group 14.

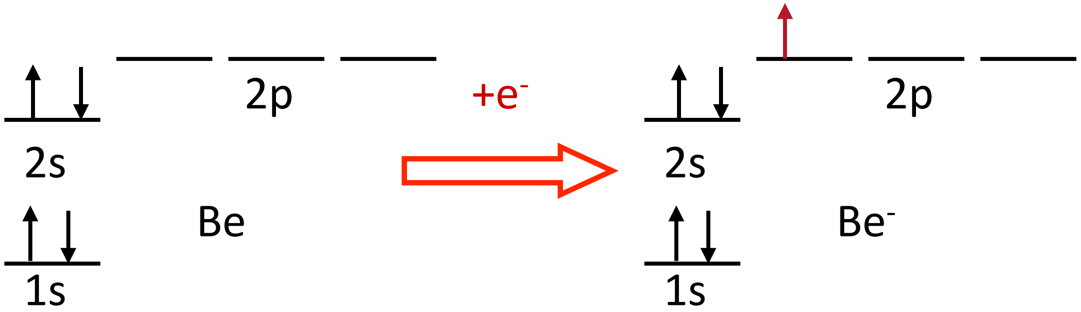
Anomalies in Electron Affinity

Noble gases and **alkaline earth metals** are the only elements to have ***positive*** electron affinity values (meaning addition of an electron ***requires*** energy – unfavourable)

WHY?

↳ the added electron must fit into a higher energy orbital
↳ this requires expenditure of energy

Alkaline earths are all ns^2:

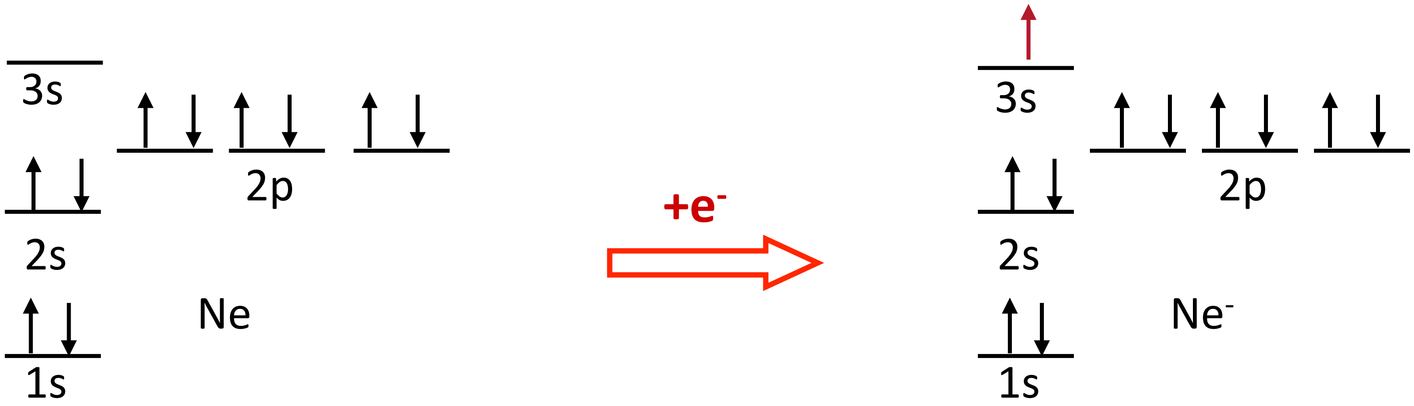


added electron must go in ***higher energy p-orbital***

Positive electron affinity (unfavourable)

Anomalies in Electron Affinity

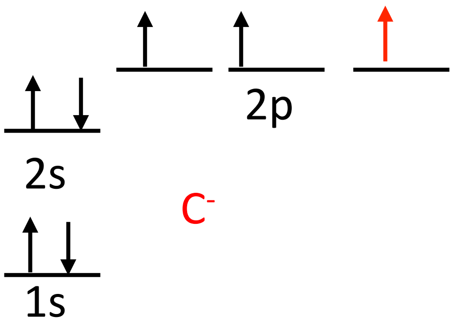
Similar reasoning applies for the **inert gases**; the added electron must go into a new principal quantum level:

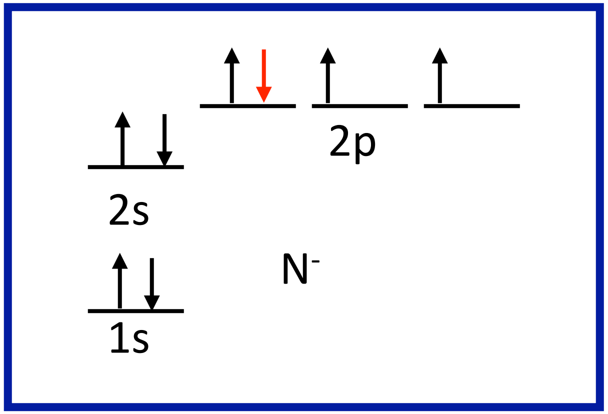


Positive electron affinity: Unfavourable

Anomalies in Electron Affinity

Adding an electron to a group 15 element is less favourable than adding an electron to a group 14 element.





Adding an electron to C (group 14) allows it to go unpaired into the one empty 2p orbital

Adding an electron to N (group 15) means that it must pair up. (Unfavourable e-e repulsion)

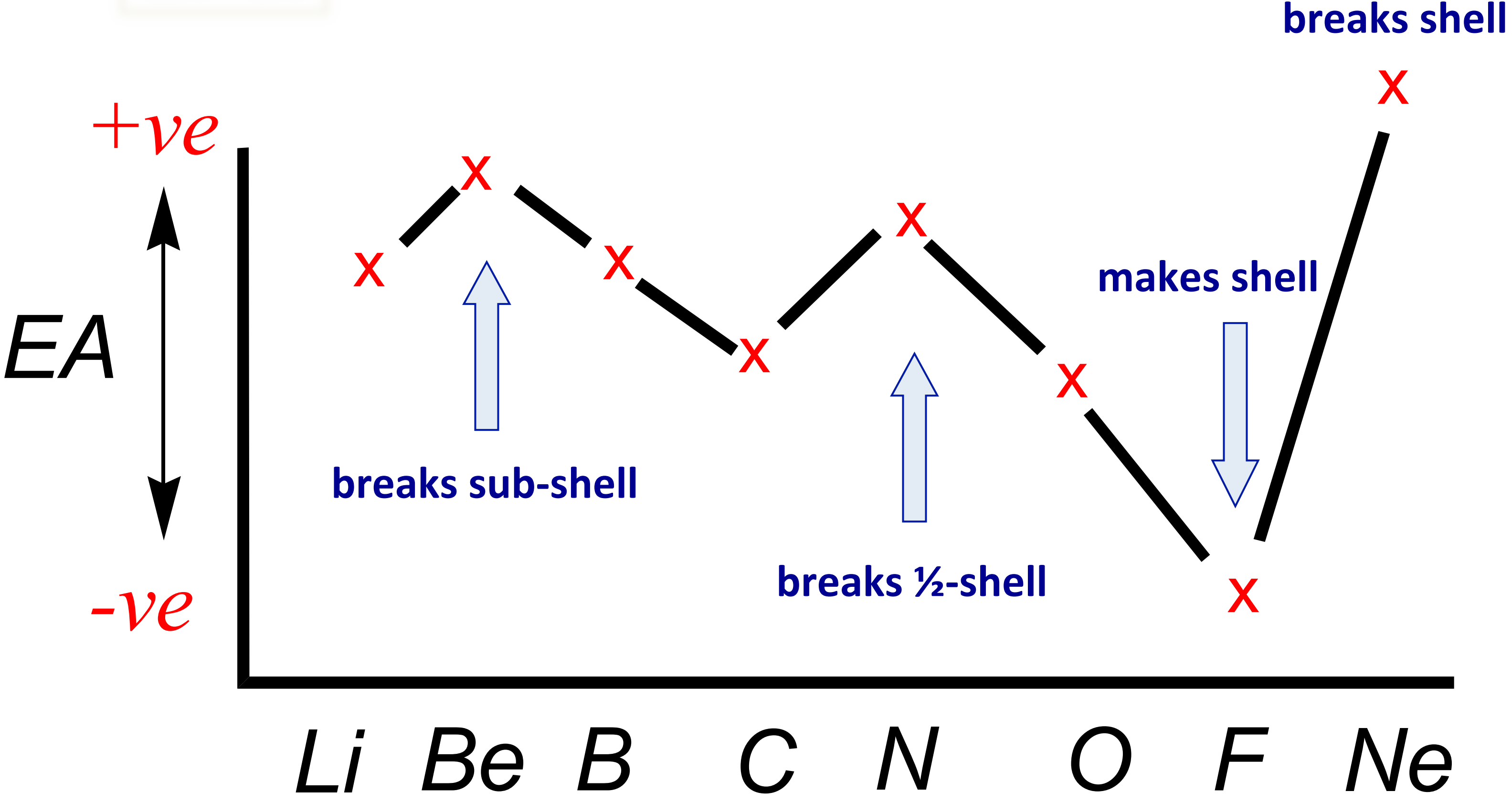
Addition of an electron to C is more favourable than addition of an electron to N

Variations in Electron Affinity

$A(g) + e \rightarrow A(g)^-$

$\Delta H = EA$

An “*electron hungry*” atom will have a large negative EA



Electron Affinity

Addition of a **2nd** electron is always ENDOTHERMIC (unfavourable)

$$X^- (g) + e^- \rightarrow X^{2-} (g)$$

A negatively charged atom has a very low Z_{eff}. An added electron will experience very little attraction to the nucleus, thus, very little stabilization.

Thus, the ***second electron affinity is always positive***

Exercise

A. Use concepts of ionization energy and electron affinity to determine which of the following is more energetically favorable:

1) adding an electron to a sodium atom

or

2) removing an electron from a sodium atom.

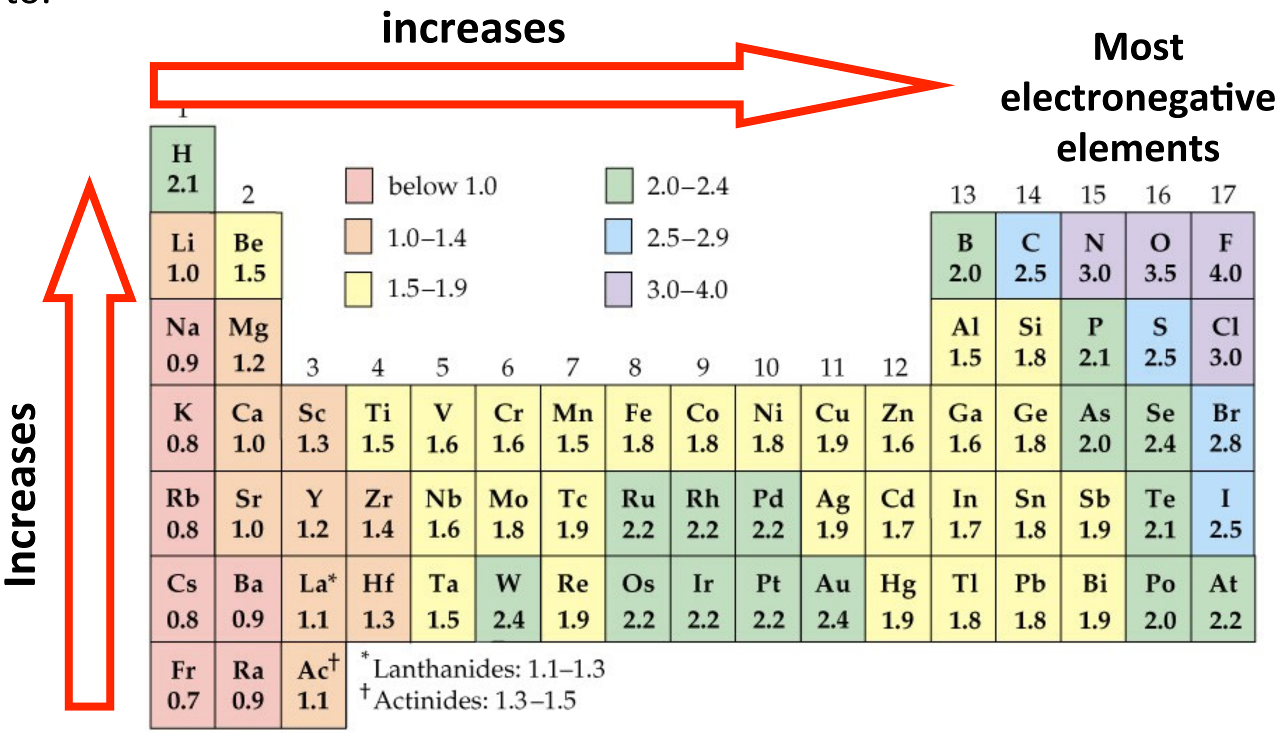
B. Is adding an electron to Si more or less favorable than adding an electron to P? Use orbital energy level diagrams to support your argument.

Electronegativity *vs* Electron Affinity

Electron affinity: ability of an ***isolated atom*** to attract an electron.

Electronegativity: the ability of an atom ***chemically bonded to another atom*** to attract the ***shared electrons***.

Electronegativity is relative*:* the electronegativity of an atom can only be determined ***relative*** to an atom that it is bonded to.



increases

Most electronegative elements

Increases

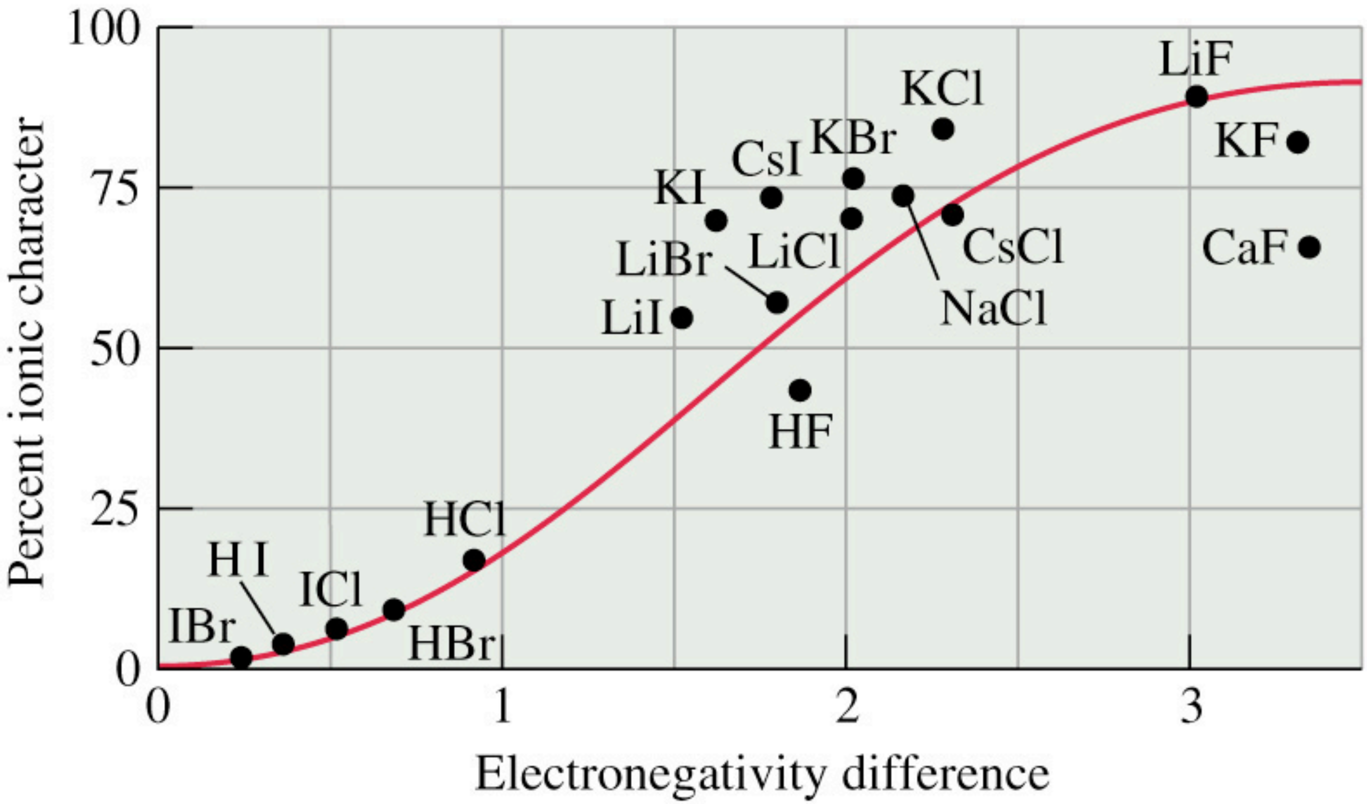
Least electronegative elements

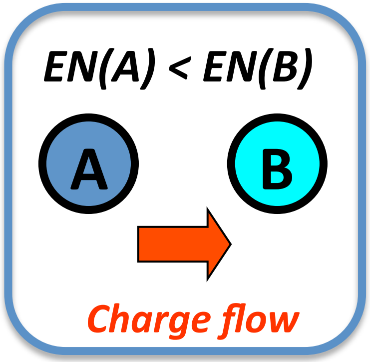
🟥 below 1.0
🟧 1.0–1.4
🟨 1.5–1.9
🟩 2.0–2.4
🟦 2.5–2.9
🟪 3.0–4.0

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
H 2.1																
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5
Cs 0.8	Ba 0.9	La* 1.1	Hf 1.3	Ta 1.5	W 2.4	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2
Fr 0.7	Ra 0.9	Ac† 1.1														

*Lanthanides: 1.1–1.3
†Actinides: 1.3–1.5

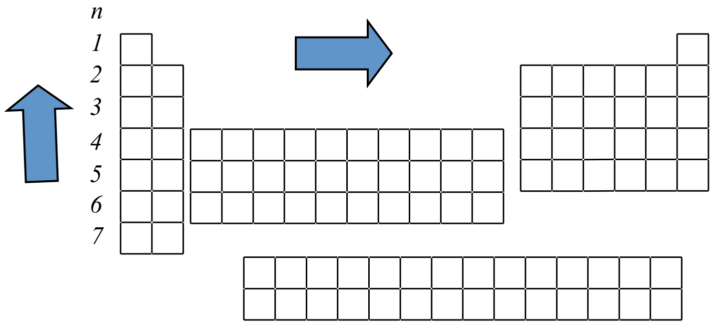
Electronegativity and Percent Ionic Character



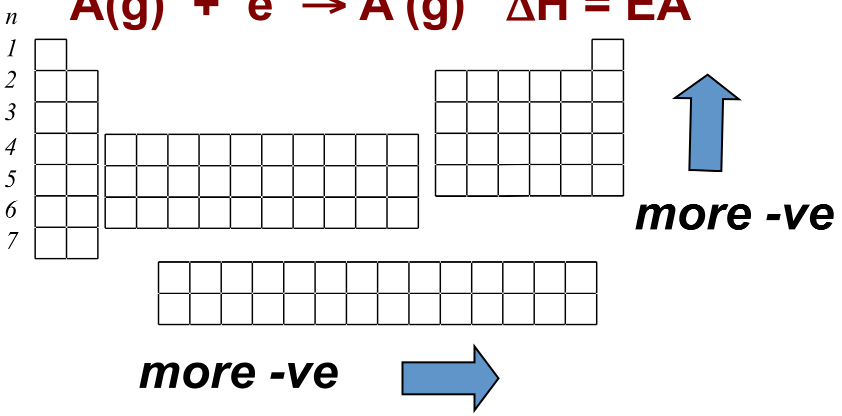


Periodic Table Trends…A Summary

$A(g) \rightarrow A^{+}(g) + e \quad \Delta H = IE$

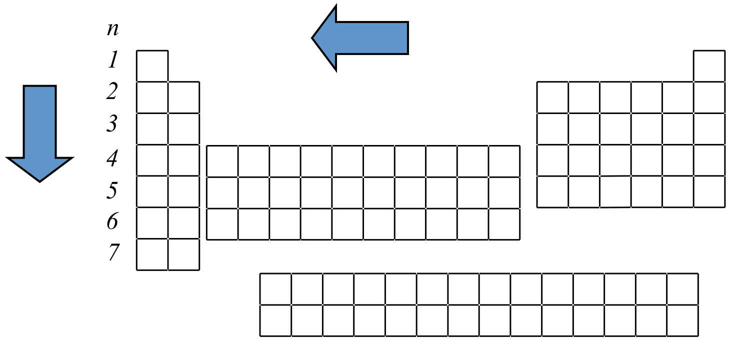


$A(g) + e \rightarrow A^{-}(g) \quad \Delta H = EA$

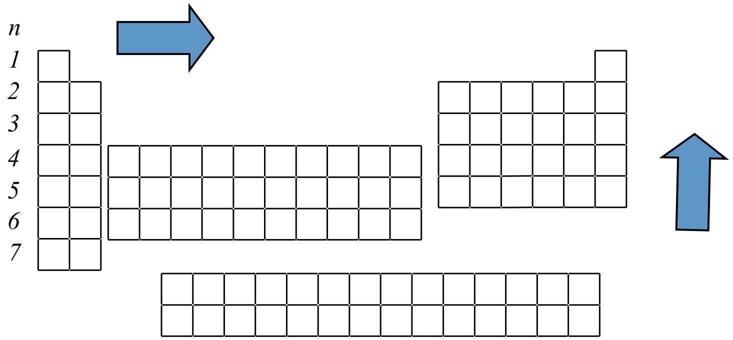


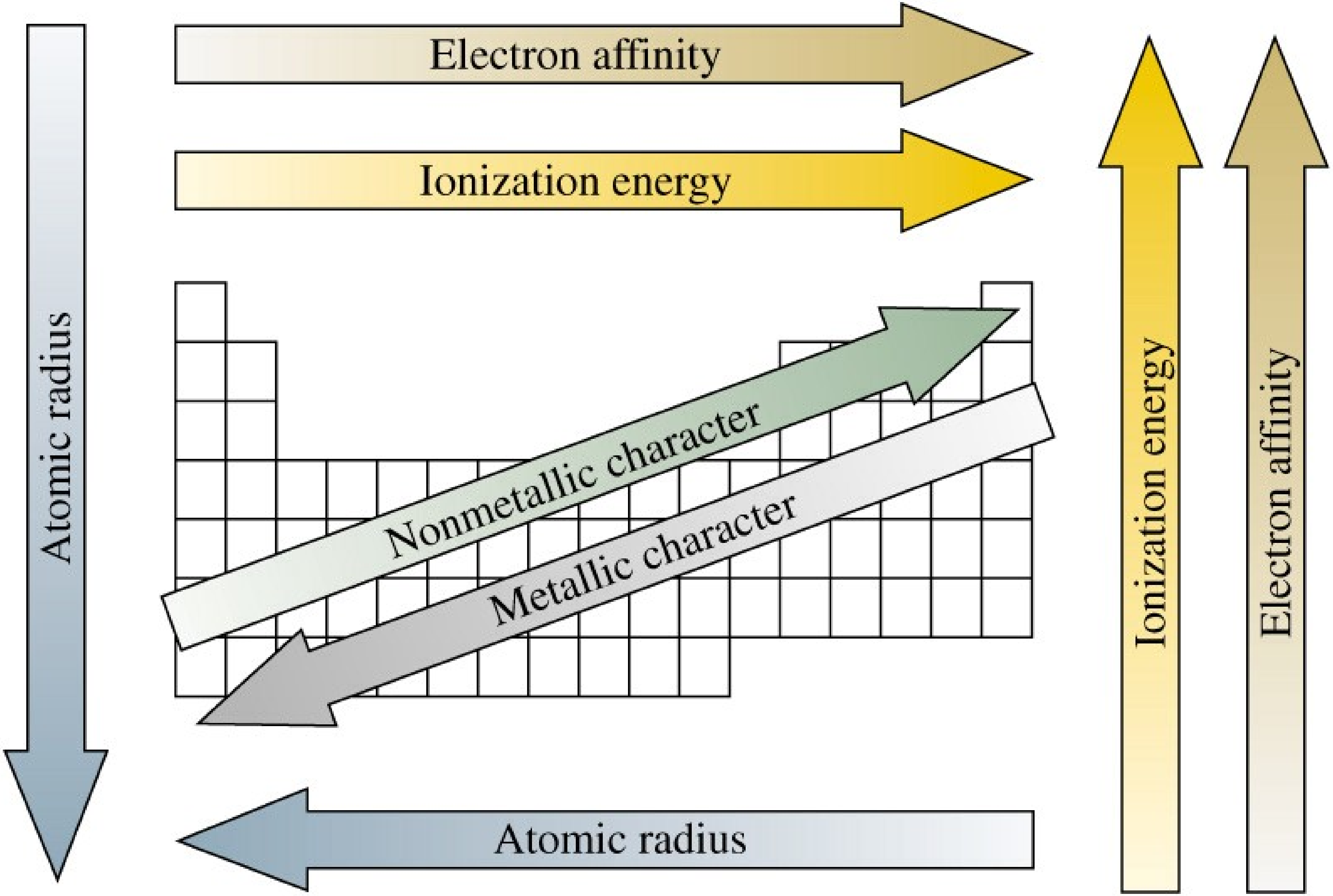
Breaking a 1/2 filled shell is extra hard, making one is extra easy

Atomic radius



Atomic electronegativity, EN




Electron affinity
Ionization energy
Atomic radius
Nonmetallic character
Metallic character
Ionization energy
Electron affinity
Atomic radius