INTERNATIONAL COLLEGE OF PHARMACEUTICAL INNOVATION
国际创新药学院

Class	Pharm, BioPharm
Course	Fundamentals of Medicinal & Pharmaceutical Chemistry
Code	FUNCHEM.4
Title	The Periodic Table: Trends and Properties
Lecturer	Prof. Xinchen Teng
Date	2024-10-11

RECOMMENDED READING

- General Chemistry - The Essential Concepts by Chang and Goldsby (7^{th} edition)
  - Sections 2.4, 8.3, 8.4, 8.5, 9.5

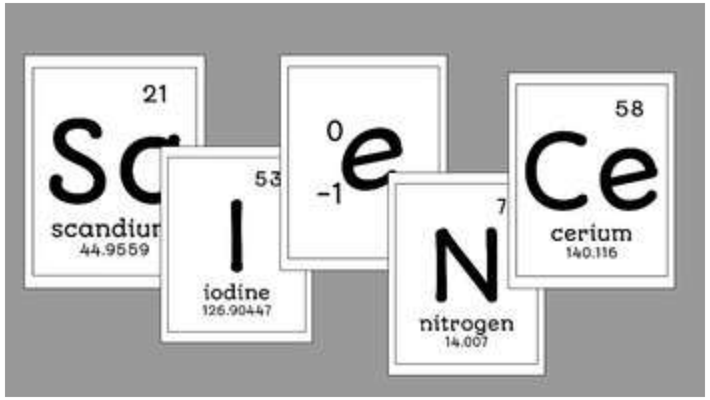
FUNCHEM.4 Learning Outcomes

- Recognise the arrangement of elements in the periodic table according to increasing atomic number.
- Differentiate between periods and groups, metals, non-metals and metalloids, alkali metals, alkaline earth metals, transition metals, halogens, inert gases, lanthanides and actinides in the periodic table.
- Define ‘effective nuclear charge’.
- Define ‘atomic radius’, ‘ionic radius’, ‘ionisation energy’, ‘electron affinity’ and ‘electronegativity’ and describe how each varies on going across a period and down a group in the Periodic Table.

The Periodic Table
(The alphabet of chemistry)

When it comes to studying the elements nature has handed us a nice simplification:

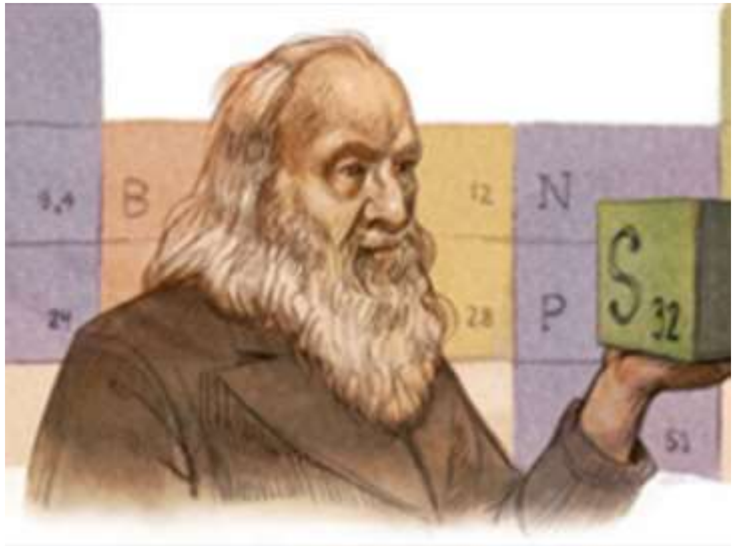
- 118 elements
- Grouped into a few families
- Displayed by the <u>Periodic Table</u>



Mendeleev’s Periodic Table

In 1869 Dmitri Mendeleev published the first arrangement of the elements

Reihen	Gruppe I. — R^2O	Gruppe II. — RO	Gruppe III. — R^2O^3	Gruppe IV. RH^4 RO^2	Gruppe V. RH^3 R^2O^5	Gruppe VI. RH^2 RO^3	Gruppe VII. RH R^2O^7	Gruppe VIII. — RO^4
1	H=1							
2	Li=7	Be=9,4	B=11	C=12	N=14	O=16	F=19	
3	Na=23	Mg=24	Al=27,3	Si=28	P=31	S=32	Cl=35,5	
4	K=39	Ca=40	—=44	Ti=48	V=51	Cr=52	Mn=55	Fe=56, Co=59, Ni=59, Cu=63.
5	(Cu=63)	Zn=65	—=68	—=72	As=75	Se=78	Br=80	
6	Rb=85	Sr=87	?Yt=88	Zr=90	Nb=94	Mo=96	—=100	Ru=104, Rh=104, Pd=106, Ag=108.
7	(Ag=108)	Cd=112	In=113	Sn=118	Sb=122	Te=125	J=127	
8	Cs=133	Ba=137	?Di=138	?Ce=140	—	—	—	— — — —
9	(—)	—	—	—	—	—	—	
10	—	—	?Er=178	?La=180	Ta=182	W=184	—	Os=195, Ir=197, Pt=198, Au=199.
11	(Au=199)	Hg=200	Tl=204	Pb=207	Bi=208	—	—	
12	—	—	—	Th=231	—	U=240	—	— — — —

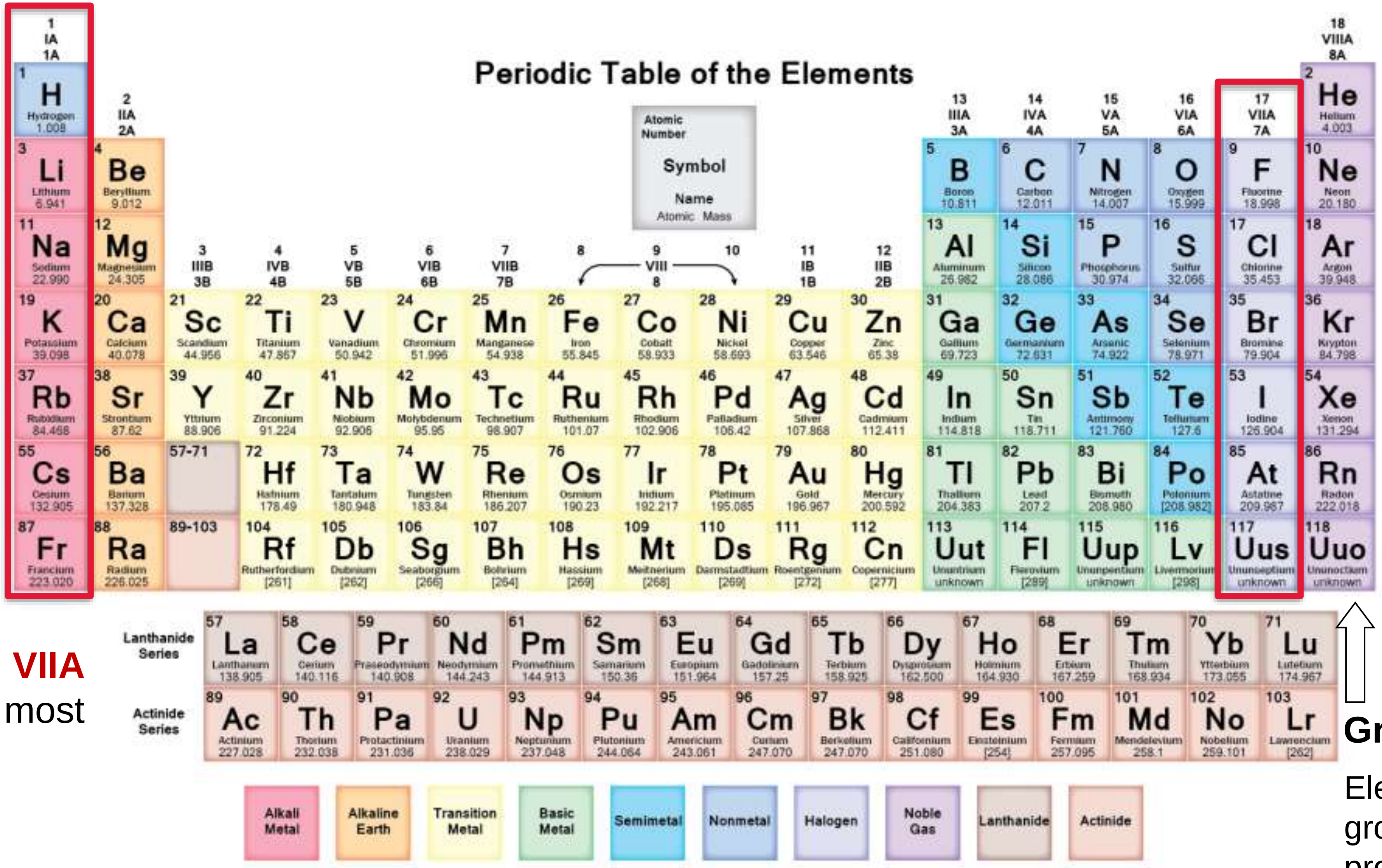


Mendeleev 1834 - 1907

- Had no idea what atoms were made of or why they behaved as they did.
- Organised the elements in order of increasing atomic mass.
- Based on gaps in his table predicted the existence and properties of several undiscovered elements.

The Modern Periodic Table

Elements represented by symbols arranged according to increasing atomic number



Periods

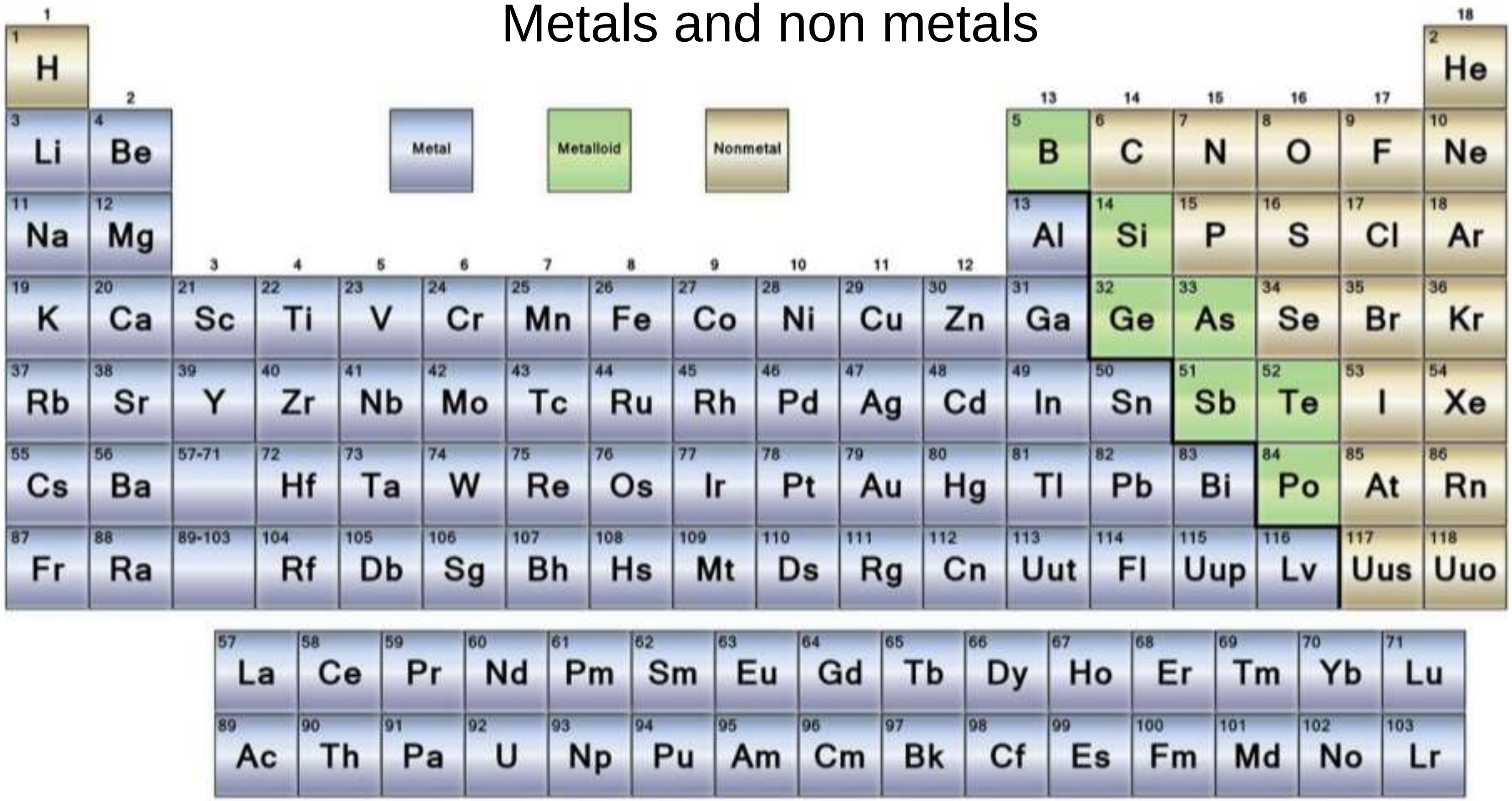
Group **IA** and **VIIA** elements are most reactive

Groups

Elements within a group show similar properties

The Modern Periodic Table

Metals and non metals



A **metal** is a good conductor of heat and electricity

A **nonmetal** is usually a poor conductor of heat and electricity

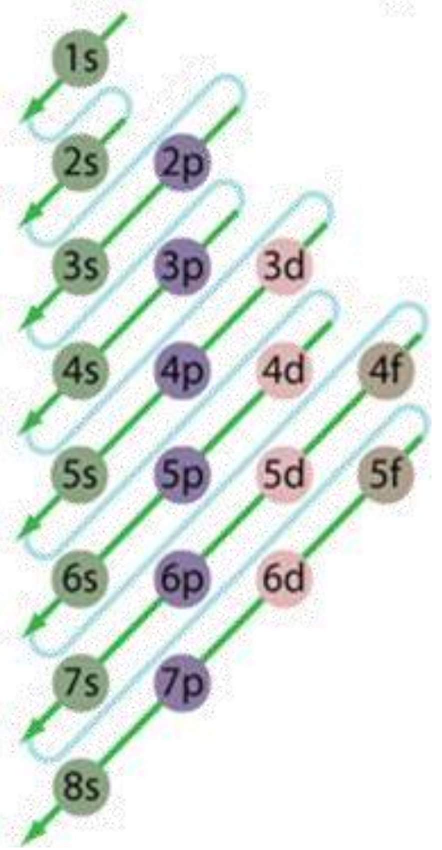
Semimetals/**Metalloid**s have properties of both metals & nonmetals

The Modern Periodic Table

Electron configuration

	1A 1	2A 2	3B 3	4B 4	5B 5	6B 6	7B 7	8B 8	8B 9	8B 10	1B 11	2B 12	3A 13	4A 14	5A 15	6A 16	7A 17	8A 18
Core	1 H $1s^1$																	2 He $1s^2$
[He]	3 Li $2s^1$	4 Be $2s^2$											5 B $2s^22p^1$	6 C $2s^22p^2$	7 N $2s^22p^3$	8 O $2s^22p^4$	9 F $2s^22p^5$	10 Ne $2s^22p^6$
[Ne]	11 Na $3s^1$	12 Mg $3s^2$											13 Al $3s^23p^1$	14 Si $3s^23p^2$	15 P $3s^23p^3$	16 S $3s^23p^4$	17 Cl $3s^23p^5$	18 Ar $3s^23p^6$
[Ar]	19 K $4s^1$	20 Ca $4s^2$	21 Sc $3d^14s^2$	22 Ti $3d^24s^2$	23 V $3d^34s^2$	24 Cr $3d^54s^1$	25 Mn $3d^54s^2$	26 Fe $3d^64s^2$	27 Co $3d^74s^2$	28 Ni $3d^84s^2$	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 $3d^{10}4s^2$ $4p^6$
[Kr]	37 Rb $5s^1$	38 Sr $5s^2$	39 Y $4d^15s^2$	40 Zr $4d^25s^2$	41 Nb $4d^35s^2$	42 Mo $4d^55s^1$	43 Tc $4d^55s^2$	44 Ru $4d^75s^1$	45 Rh $4d^85s^1$	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 $4d^{10}5s^2$ $5p^6$
[Xe]	55 Cs $6s^1$	56 Ba $6s^2$	71 Lu $4f^{14}5d^1$ $6s^2$	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 $4f^{14}5d^7$ $6s^2$	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 $4f^{14}5d^{10}$ $6s^26p^1$	82 Pb $4f^{14}5d^{10}$ $6s^26p^2$	83 Bi $4f^{14}5d^{10}$ $6s^26p^3$	84 Po $4f^{14}5d^{10}$ $6s^26p^4$	85 At $4f^{14}5d^{10}$ $6s^26p^5$	86 Rn $4f^{14}5d^{10}$ $6s^26p^6$
[Rn]	87 Fr $7s^1$	88 Ra $7s^2$	103 Lr $5f^{14}6d^1$ $7s^2$	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	111	112						

[Xe] Lanthanide series	57 La $5d^16s^2$	58 Ce $4f^15d^1$ $6s^2$	59 Pr $4f^36s^2$	60 Nd $4f^46s^2$	61 Pm $4f^56s^2$	62 Sm $4f^66s^2$	63 Eu $4f^76s^2$	64 Gd $4f^75d^1$ $6s^2$	65 Tb $4f^96s^2$	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 $4f^{14}6s^2$
[Rn] Actinide series	89 Ac $6d^17s^2$	90 Th $6d^27s^2$	91 Pa $5f^26d^1$ $7s^2$	92 U $5f^36d^1$ $7s^2$	93 Np $5f^46d^1$ $7s^2$	94 Pu $5f^67s^2$	95 Am $5f^77s^2$	96 Cm $5f^76d^1$ $7s^2$	97 Bk $5f^97s^2$	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 $5f^{14}7s^2$

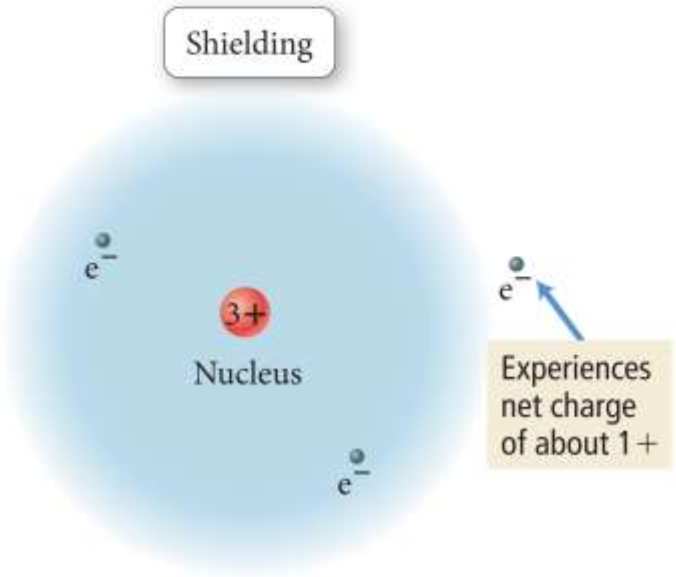


Valence electrons

The outmost or valence shell electrons are very important because they participate in the sharing and exchange that is responsible for chemical reactions

The attraction between the positive nucleus and the outermost negative electrons (valence electron) depends on:

1. Number of protons in the nucleus
2. Shielding effect of other e^- closer to nucleus
3. Distance form the nucleus



Effective Nuclear Charge, Z_{eff}

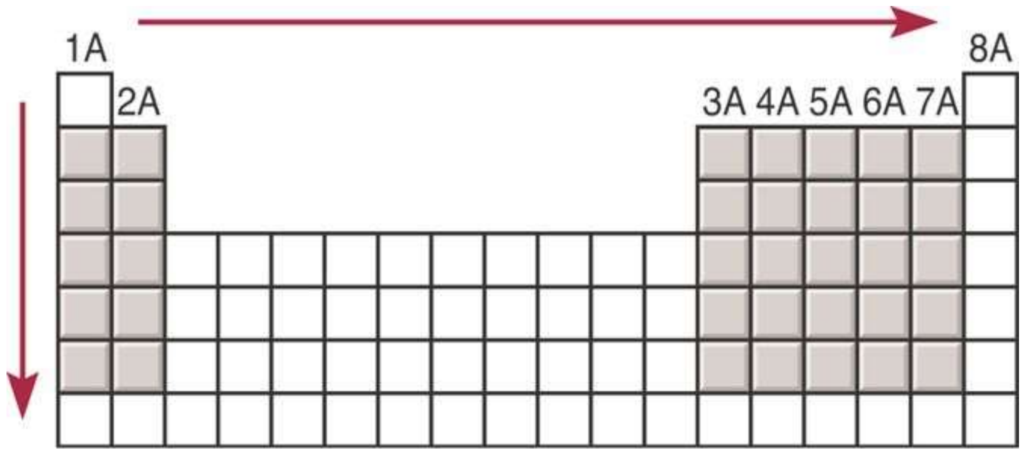
The **effective nuclear charge (Z_{eff})** is the nuclear charge felt by an electron when both the actual nuclear charge (Z) and the repulsive effects (shielding) of the other electrons are taken into account.

$$Z_{eff} = Z - \sigma$$

σ (sigma) is called the *shielding constant* (also called the *screening constant*). The shielding constant is greater than zero but smaller than *Z.*

From left to right, **Z_{eff} increases**
Z increases, the added electron is a valence electron and valence electrons do not shield each other well, greater effective nuclear charge felt by the valence electrons.

Going Down
Z_{eff} increases as calculated per Slaters rules
Slaters rules calculates σ by accounting for the effective shielding of electrons in each orbital "shell".



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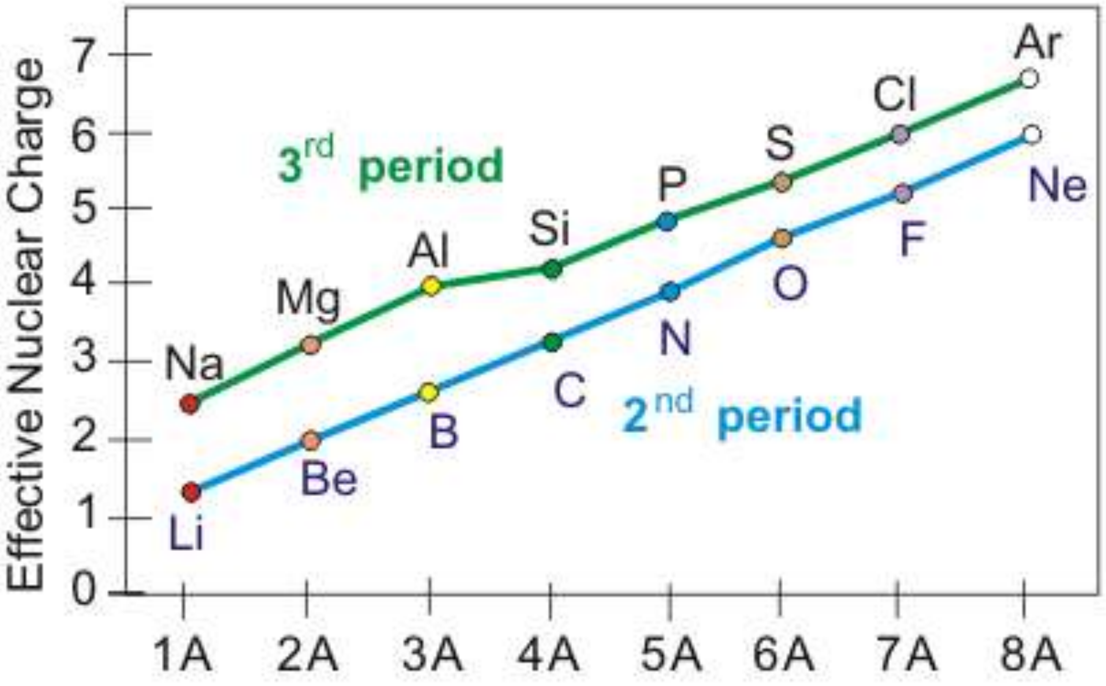
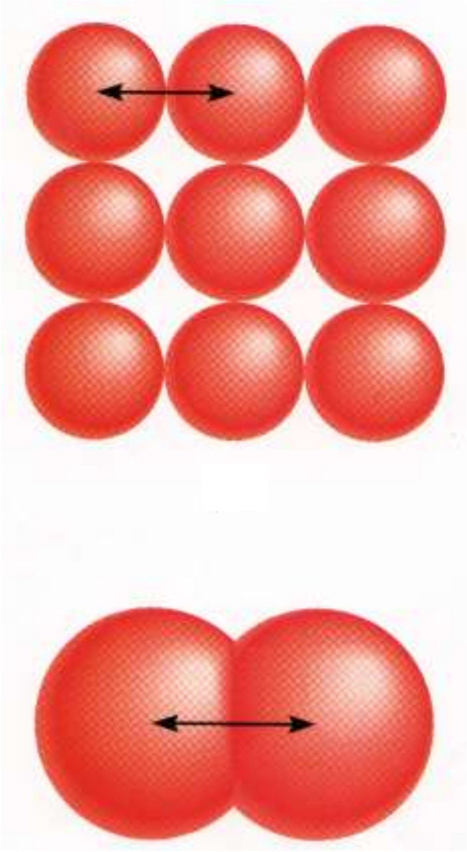
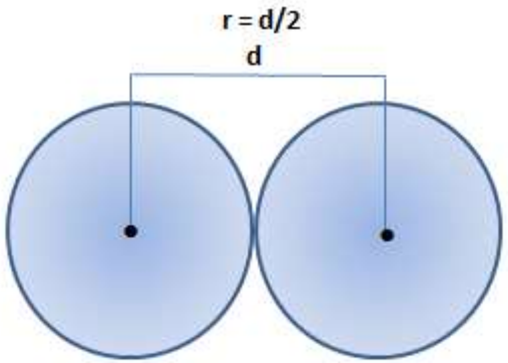


Atomic Radius

The **atomic radius** of an element is half the distance between the nuclei of two adjacent atoms



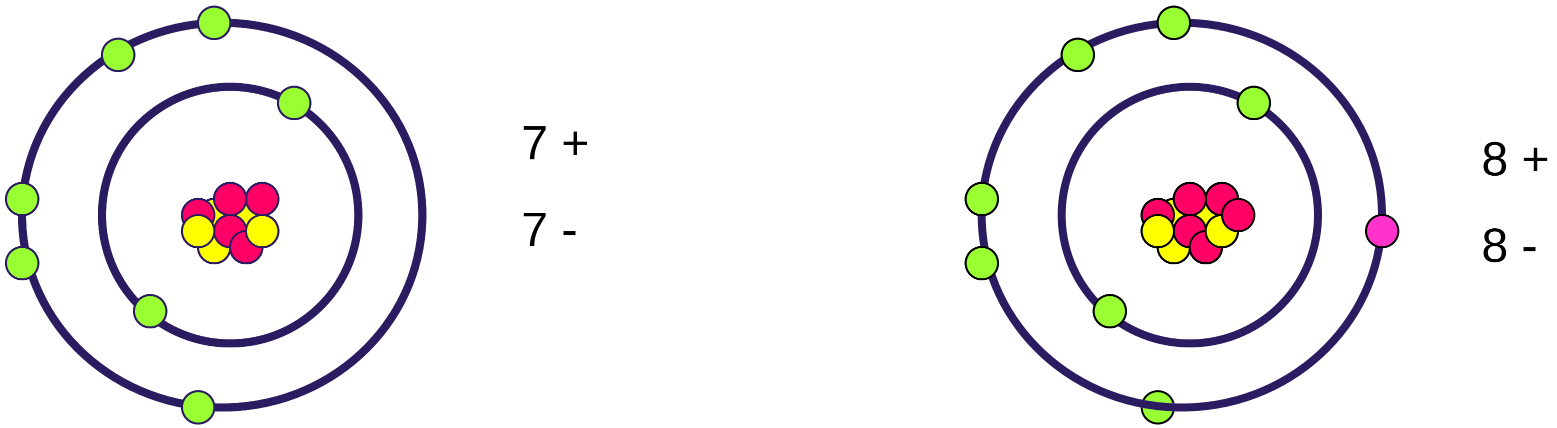


<u>How does the atomic radius vary</u>

- On going across a period?
- On going down a group?

Atomic Radius

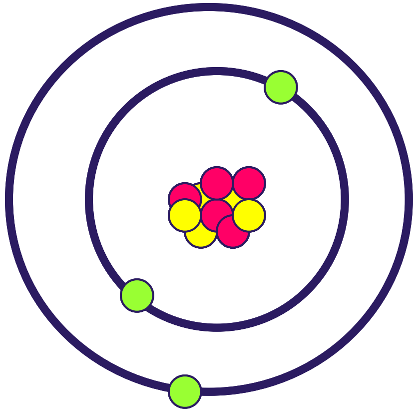
On going across a period

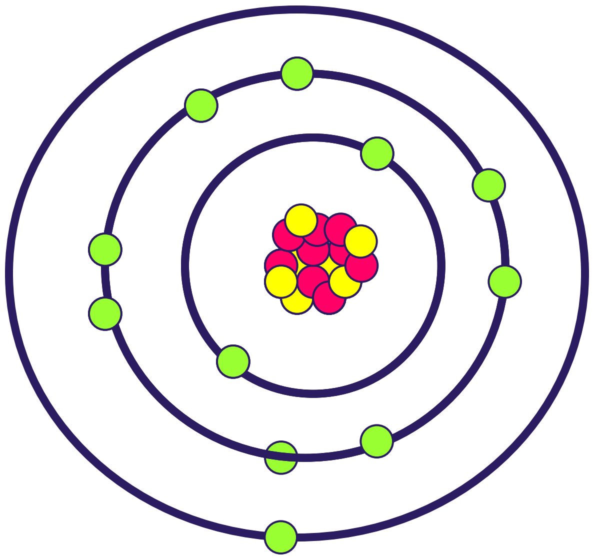


- Increasing atomic number, Z, therefore increasing number of protons in nucleus
- Adding e^- to same energy level, not very much sheilding
- Effective nuclear charge, Z_{eff}, increases
- Bigger attraction
- **Atomic radius <u>decreases</u>**

Atomic Radius

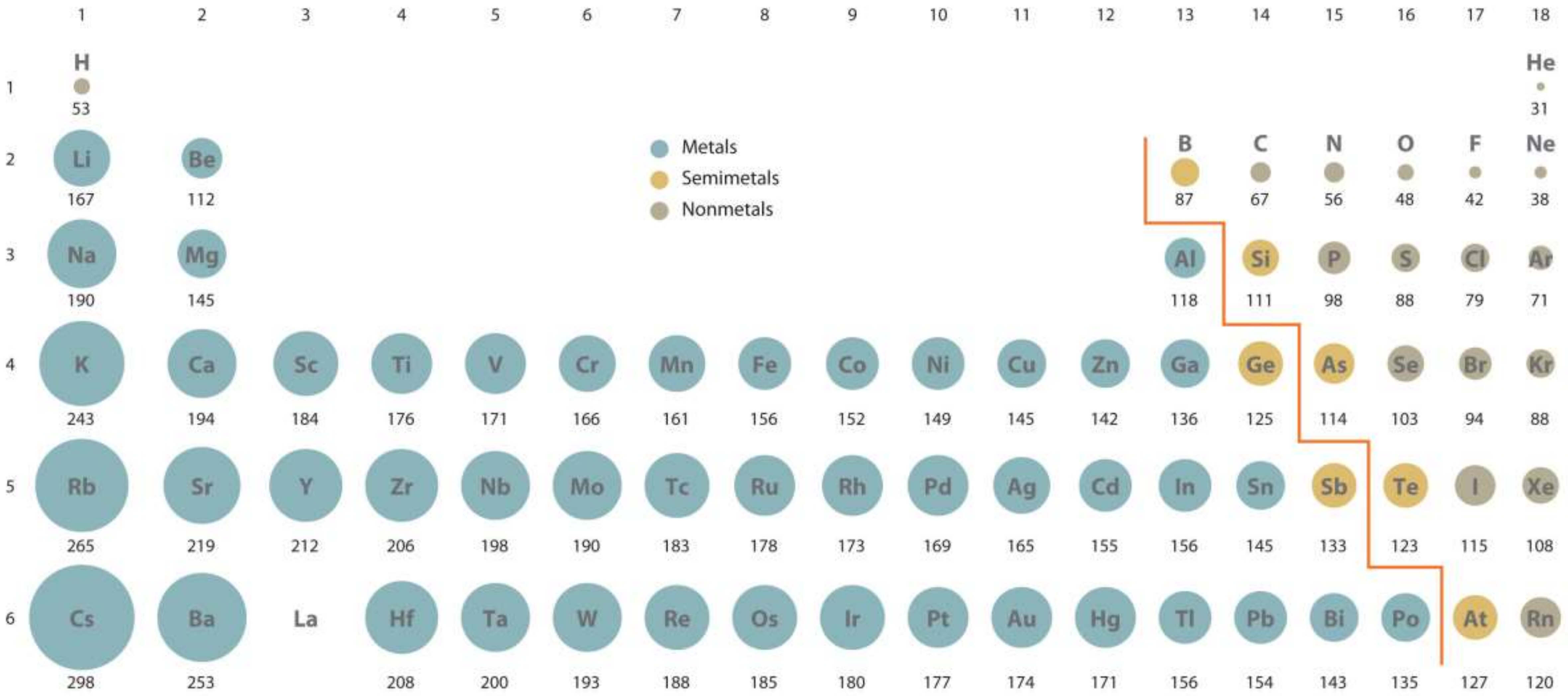
On going down a group





- Electrons enter another energy level
- A greater distance between the nucleus and outermost shell
- Electrons added in filled inner shells have high shielding effect
- **Atomic radius <u>increases</u>**

Atomic Radius



Ionic Radius

Radius of a cation or an anion

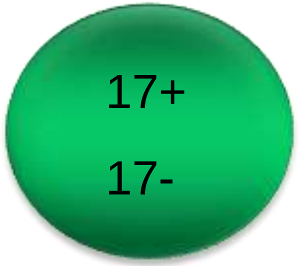
Formation of an anion (X^-)

Additional electron(s)

- Nuclear charge remains the same
- Greater repulsion amongst electrons

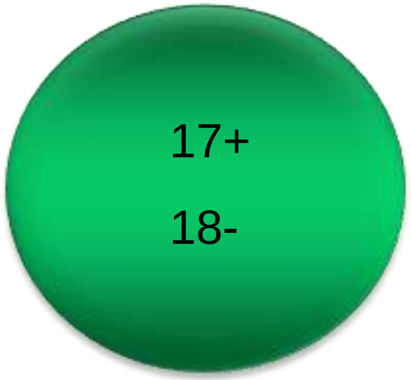
Size increases
i.e. ionic radius increases

Cl atom



99 pm

Cl^- ion



181 pm

Ionic Radius

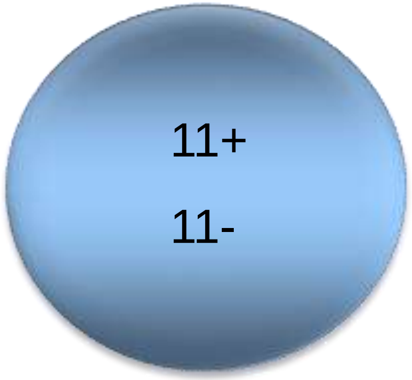
Radius of a cation or an anion

Formation of a cation (X^+)

- Less electron(s)
- Nuclear charge remainsnthe same
- Less repulsion amongst electrons

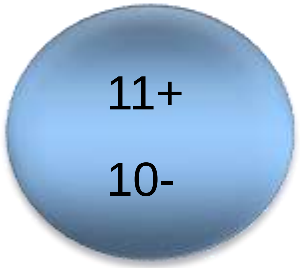
Size decreases
i.e. ionic radius decreases

Na atom



186 pm
$1s^2\ 2s^2\ 2p^6\ 3s^1$

Na^+ ion



99 pm

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

Ionic Radius

Radius of Dipositive Ion < Radius of Unipositive Ion

Why?

$_{11}Na \rightarrow Na^+$

11+	11+
11-	10 -

$_{12}Mg \rightarrow Mg^{2+}$

12+	12+
12-	10 -

Na^+ and Mg^{2+} are isoelectronic
Mg^{2+} has Bigger nuclear charge
Bigger attraction
Smaller size

Ionic Radius

Which is larger?

O^{2-} or F^{-}

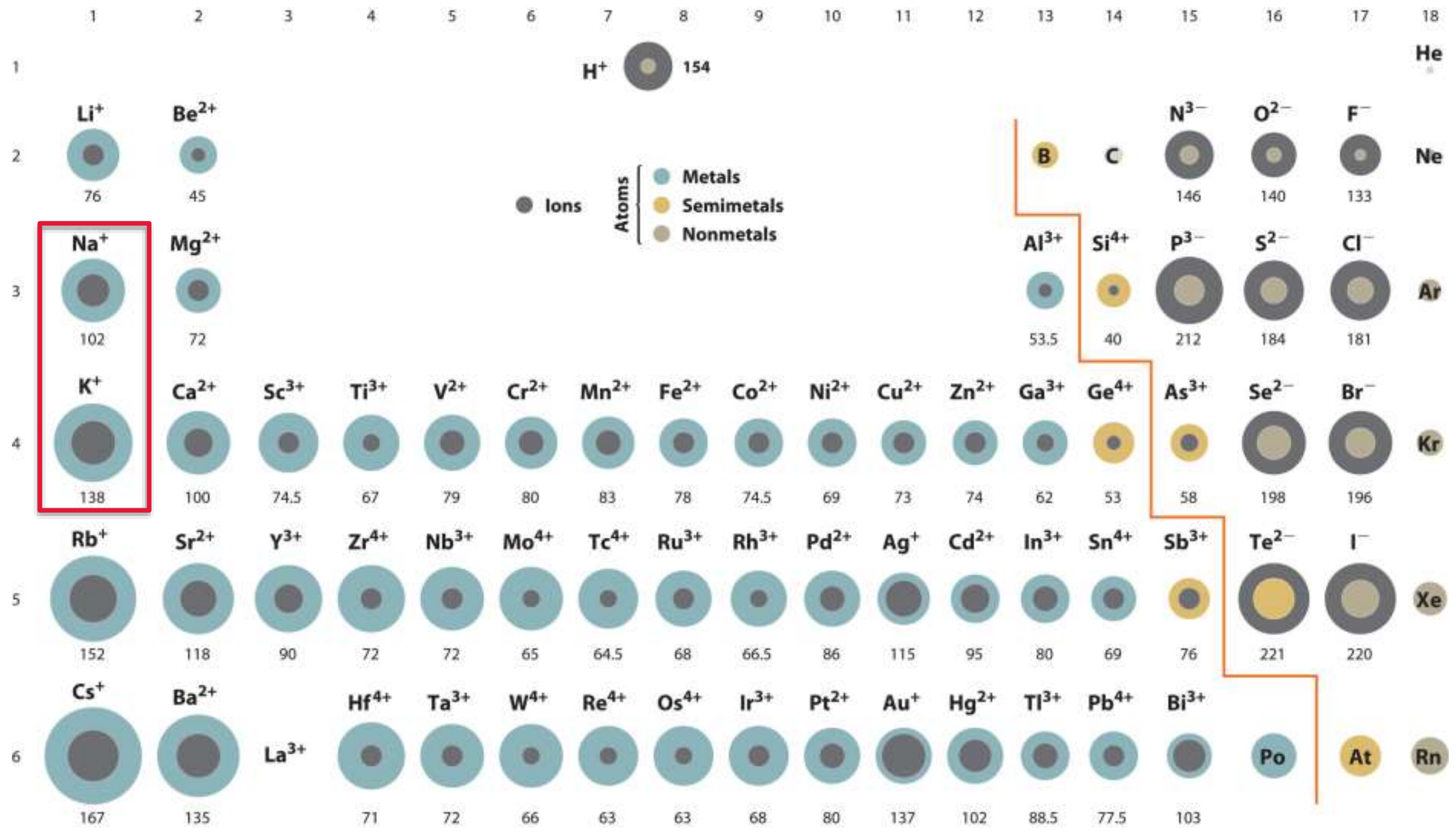
Radius of a dinegative ion > radius of a uninegative ion

O^{2-} and F^{-} are isoelectronic
F^{-} has bigger nuclear charge
Bigger attraction
Smaller size

Watch the animation titled ‘Atomic and Ionic Radius’ on the VLE

Ionic Radius

Ions move through tiny channels in cell membranes.
Some channels allow Na^+ through but not larger K^+



Ionisation Energy

Electrons are attracted to the positive charge in the nucleus.
Energy is needed to overcome this attraction.

Ionization energy (IE) is the minimum energy (in kJ/mol) required to remove an electron from a gaseous atom in its ground state.

First Ionisation Energy (IE_1)

$M_{(g)} + IE_1 \longrightarrow M^{+}_{(g)} + e^-$ (removal of first electron)

Second Ionisation Energy (IE_2)

$M^{+}_{(g)} + IE_2 \longrightarrow M^{2+}_{(g)} + e^-$ (removal of second electron)

Third Ionisation Energy (IE_3)

$M^{2+}_{(g)} + IE_3 \longrightarrow M^{3+}_{(g)} + e^-$ (removal of third electron)

Ionisation Energy

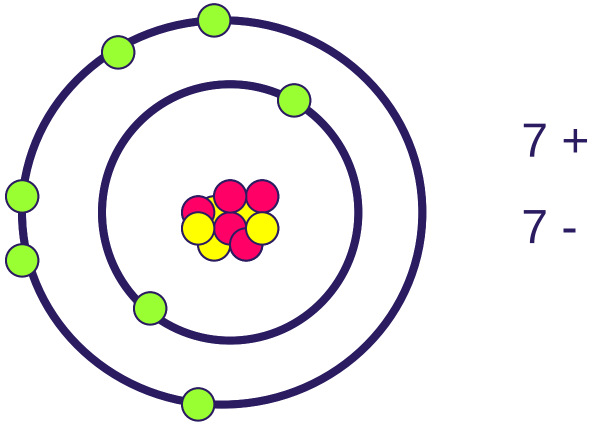
The ionization energy increases dramatically after all the outer electrons are removed. The inner electrons in the core are too tightly bound to the nucleus.

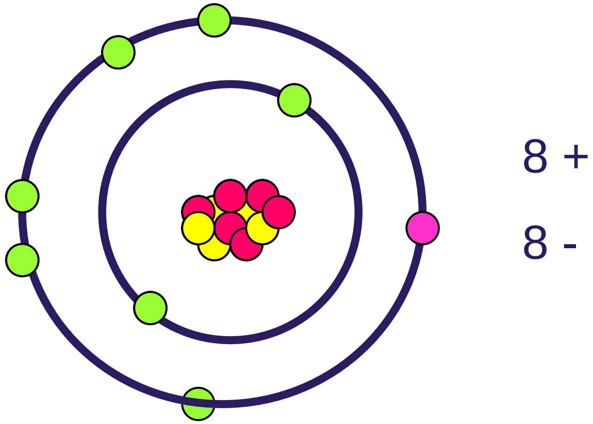
Successive Ionization Energies for Period 2 Elements (kJ/mol)

Element	IE_1	IE_2	IE_3	IE_4	IE_5	IE_6	IE_7	IE_8	IE_9	IE_{10}
Li	520	7298	11,815							
Be	899	1757	14,849	21,006		Core electrons				
B	800	2427	3660	25,026	32,827					
C	1086	2353	4620	6222	37,830	47,277				
N	1402	2856	4582	7475	9445	53,266	64,360			
O	1314	3388	5300	7469	10,989	13,326	71,334	84,078		
F	1681	3374	6050	8408	11,023	15,164	17,868	92,038	106,434	
Ne	2080	3952	6122	9370	12,178	15,238	19,999	23,069	115,379	131,431

Ionisation Energy

On Going Across A Period

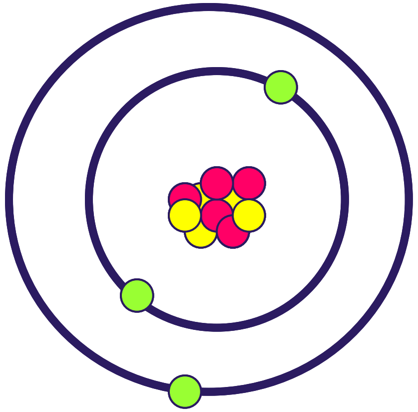




- Nuclear Charge, Z, increases
- Adding e^- to same energy level
- Effective nuclear charge, Zeff, increases
- Bigger attraction
- **Ionisation energy <u>increases</u>**

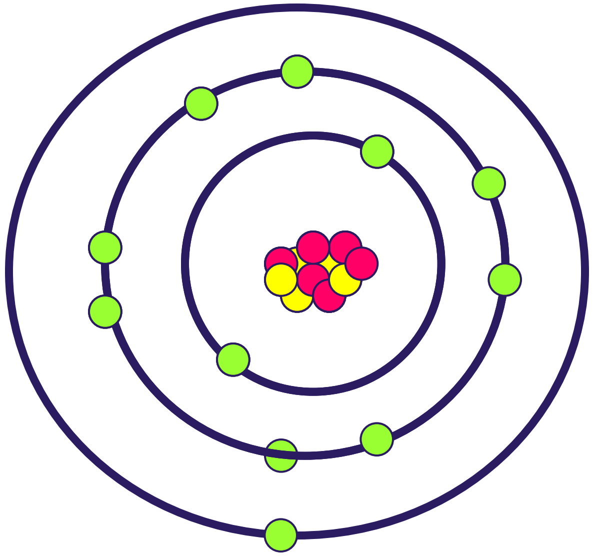
Ionisation Energy

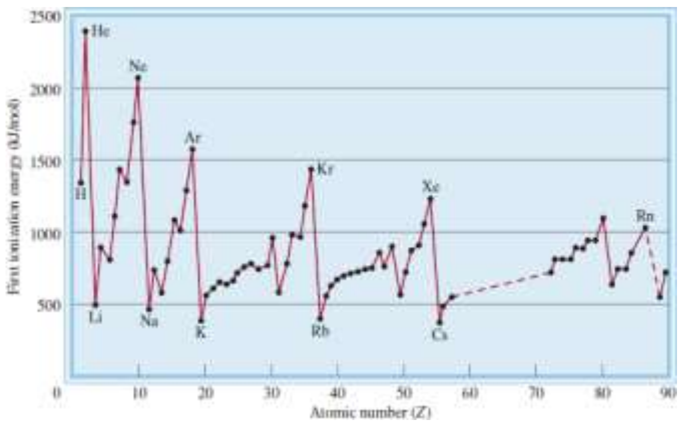
On Going Down A Group



- Electrons enter another energy level

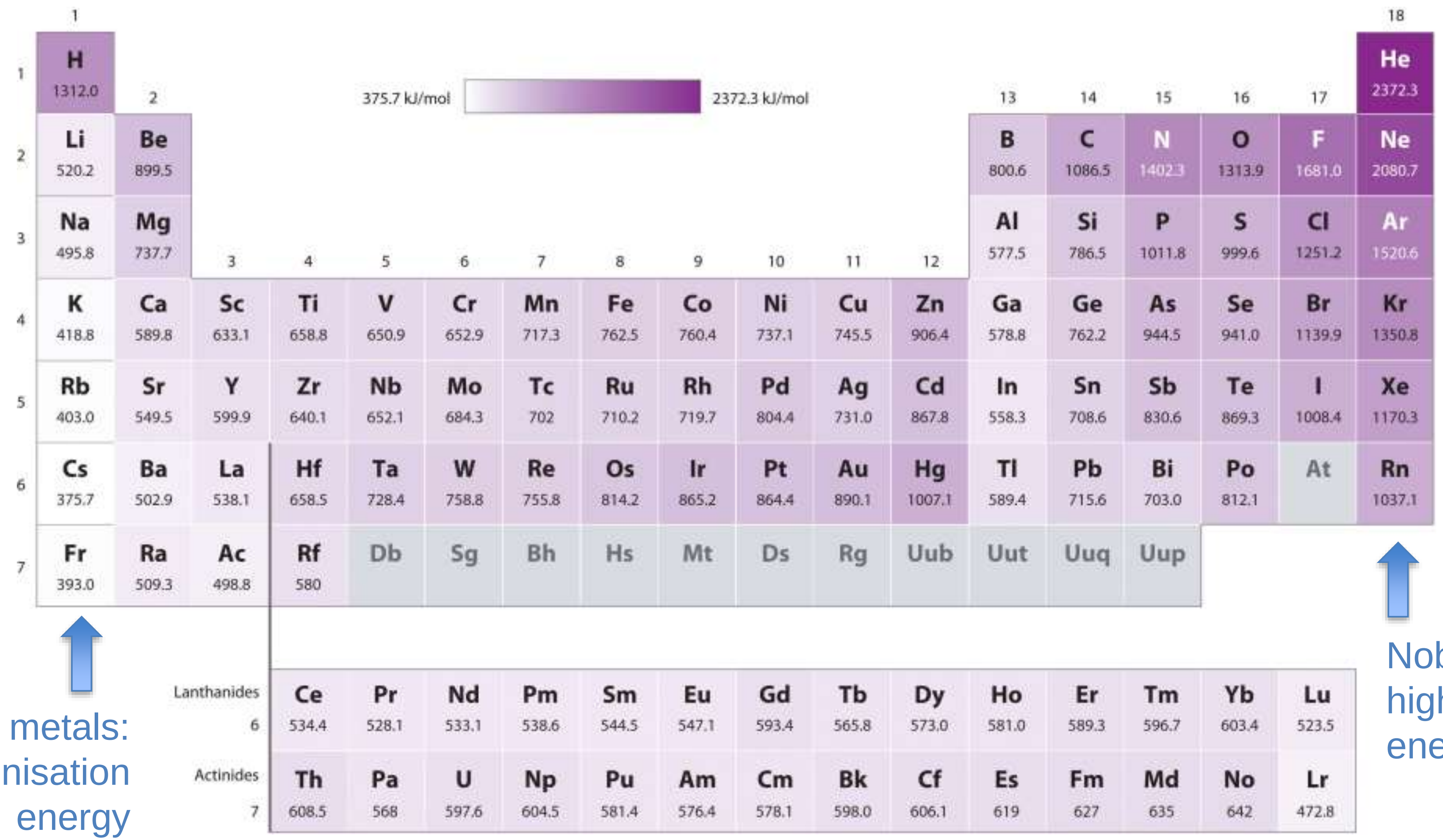
  i.e. greater distance between nucleus and outermost shell and outermost e^-
- The increased distance weakens the nuclear attraction to the outermost e^-
- **Ionisation energy <u>decreases</u>**





Ionisation Energy

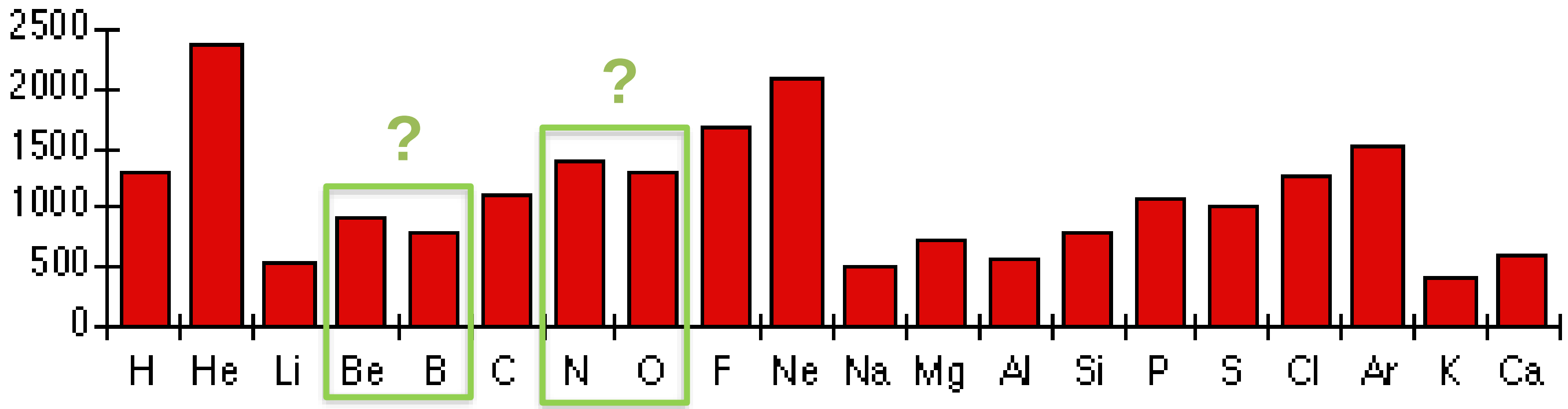
In general, the bigger the atom, the less ionization energy and vice versa.

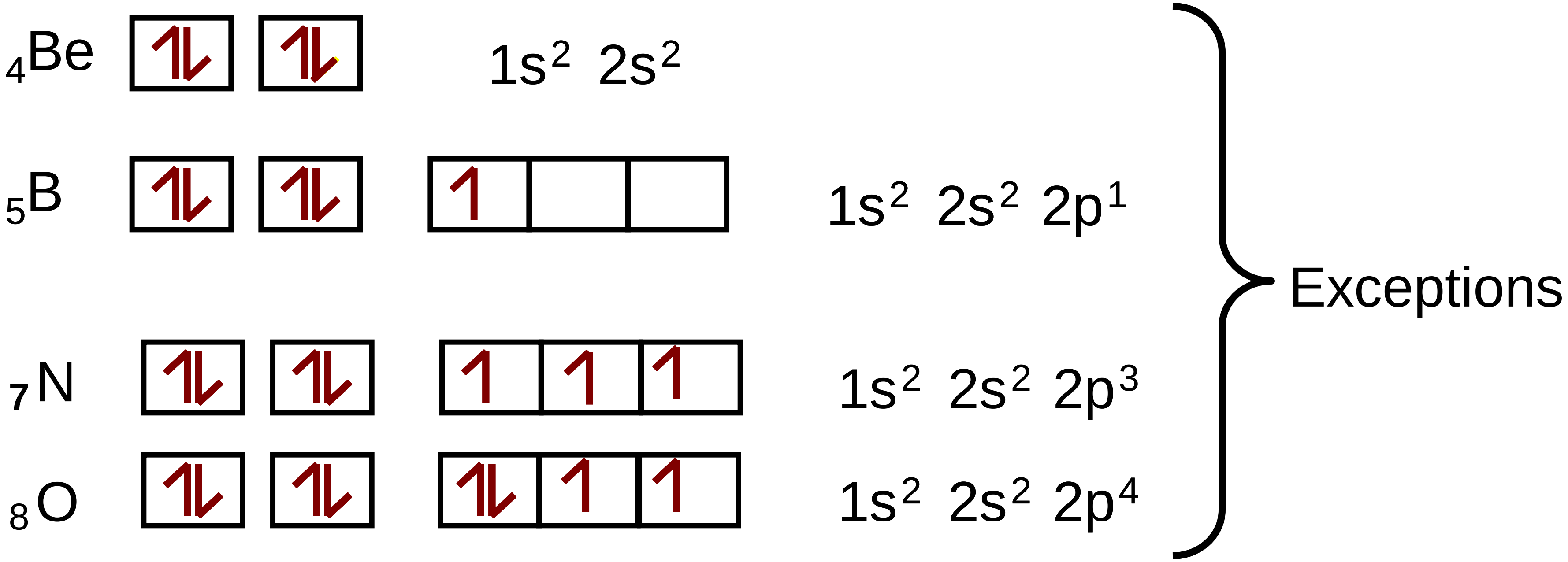


Alkali metals: lowest ionisation energy

Noble gases: highest ionisation energy

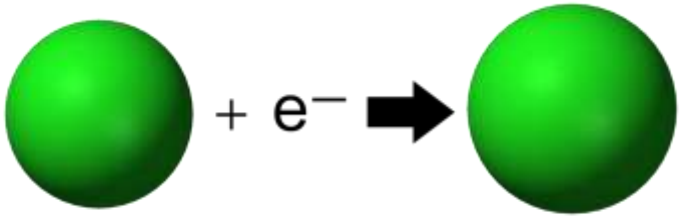
Ionisation Energy





Electron Affinity

$$X_{(g)} \quad + \quad e^- \longrightarrow X^-_{(g)}$$



Electron affinity (EA) is the **negative** of the energy change that occurs when an electron is accepted by an atom in the gaseous state to form an anion.

The more positive the electron affinity of an element,
the greater is the affinity of an atom of the element to accept an electron.

$$F_{(g)} \quad + \quad e^- \longrightarrow F^-_{(g)} \quad \Delta H = -\ 328\ kJ\ mol^{-1}$$

When ΔH is negative,
energy is released

Electron affinity is + 328 KJ mol^{-1}

Electron Affinity

≥0 kJ/mol — +348.6 kJ/mol

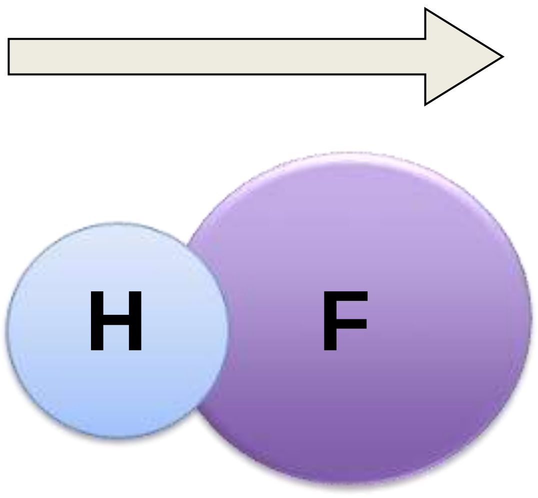
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H +72.8																	He ≤0
2	Li +59.6	Be ≤0											B +27.0	C +121.8	N ≤0	O +141.0	F +328.2	Ne ≤0
3	Na +52.9	Mg ≤0											Al +41.8	Si +134.1	P +72.0	S +200.4	Cl +348.6	Ar ≤0
4	K +48.4	Ca +2.4	Sc +18	Ti +8	V +51	Cr +65.2	Mn ≥0	Fe +15	Co +64.0	Ni +111.7	Cu +119.2	Zn ≤0	Ga +40	Ge +118.9	As +78	Se +195.0	Br +324.5	Kr ≤0
5	Rb +46.9	Sr +5.0	Y +30	Zr +41	Nb +86	Mo +72.1	Tc +60	Ru +101.0	Rh +110.3	Pd +54.2	Ag +125.9	Cd ≤0	In +39	Sn +107.3	Sb +101.1	Te +190.2	I +295.2	Xe ≤0
6	Cs +45.5	Ba +14.0	La +45	Hf ≤0	Ta +31	W +79	Re +20	Os +104.0	Ir +150.9	Pt +205.0	Au +222.7	Hg ≤0	Tl +37	Pb +35	Bi +90.9	Po +180	At +270	Rn ≤0
7	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Uub	Uut	Uuq	Uup			

Lanthanides 6	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Actinides 7	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Electronegativity

H : F

Electrons in a bond rarely get shared equally.



Electronegativity

Electronegativity, the ability of an atom to attract toward itself the electrons in a chemical bond

H : H Electrons in the bond shared equally

H : F F more electronegative than H
F pulls e^- towards itself

$\delta+$ H — F $\delta-$

slight gain of e^-

H — F

movement of e^- towards F
Dipole

Electronegativity

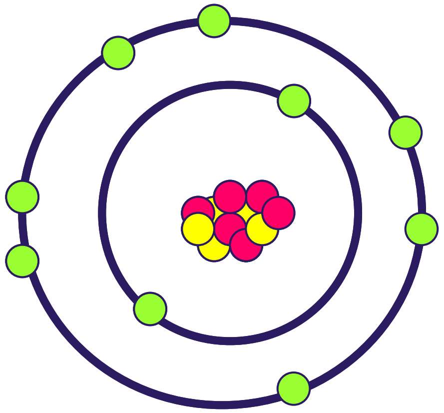
0.7 3.98

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H 2.20																	He
2	Li 0.98	Be 1.57											B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne
3	Na 0.93	Mg 1.31											Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar
4	K 0.82	Ca 1.00	Sc 1.36	Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr
5	Rb 0.82	Sr 0.95	Y 1.22	Zr 1.33	Nb 1.6	Mo 2.16	Tc 2.10	Ru 2.2	Rh 2.28	Pd 2.20	Ag 1.93	Cd 1.69	In 1.78	Sn 1.96	Sb 2.05	Te 2.1	I 2.66	Xe
6	Cs 0.79	Ba 0.89	La 1.10	Hf 1.3	Ta 1.5	W 1.7	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	Rn
7	Fr 0.7	Ra 0.9	Ac 1.1	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Uub	Uut	Uuq	Uup			

Lanthanides 6	Ce 1.12	Pr 1.13	Nd 1.14	Pm	Sm 1.17	Eu	Gd 1.20	Tb	Dy 1.22	Ho 1.23	Er 1.24	Tm 1.25	Yb	Lu 1.0
Actinides 7	Th 1.3	Pa 1.5	U 1.7	Np 1.3	Pu 1.3	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Why is F the most electronegative element?

$_{9}F$



- High nuclear charge
- Little shielding

- Electronegativity is related to electron affinity and ionization energy.
- Fluorine has a high electron affinity (tends to pick up electrons easily)
- Fluorine has a high ionization energy (does not lose electrons easily)

F > O > N > C

‘**F**ront **O**ffice **N**ever **C**loses’

Periodic Table Trends