

Periodic Table

Effective nuclear charge

The **effective nuclear charge** is the actual amount of positive (nuclear) charge experienced by an electron in a polyelectronic atom.

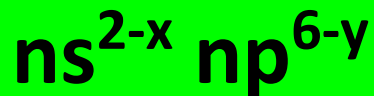
The term "effective" is used because the shielding effect of negatively charged electrons prevent higher orbitals from experiencing the full nuclear charge of the nucleus.

# The main group elements

s block element

p block element

																		18 VIIIA	
																		2 He Helium 4.002602	
																		10 Ne Neon 20.1797	
																		18 Ar Argon 39.948	
																		36 Kr Krypton 83.798	
																		54 Xe Xenon 131.293	
																		86 Rn Radon (222)	
																		118 Og Oganesson (294)	



# The noble family

1 1A	2 IIA											13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1 <b>H</b> Hydrogen 1.008												5 <b>B</b> Boron 10.81	6 <b>C</b> Carbon 12.011	7 <b>N</b> Nitrogen 14.007	8 <b>O</b> Oxygen 15.999	9 <b>F</b> Fluorine 18.998403163	2 <b>He</b> Helium 4.002602
3 <b>Li</b> Lithium 6.94	4 <b>Be</b> Beryllium 9.0121831											13 <b>Al</b> Aluminium 26.9815385	14 <b>Si</b> Silicon 28.085	15 <b>P</b> Phosphorus 30.973761998	16 <b>S</b> Sulfur 32.06	17 <b>Cl</b> Chlorine 35.45	10 <b>Ne</b> Neon 20.1797
11 <b>Na</b> Sodium 22.98976928	12 <b>Mg</b> Magnesium 24.305	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8 VIIB	9 VIIB	10 VIIB	11 IB	12 IIB						18 <b>Ar</b> Argon 39.948
19 <b>K</b> Potassium 39.0983	20 <b>Ca</b> Calcium 40.078	21 <b>Sc</b> Scandium 44.955908	22 <b>Ti</b> Titanium 47.867	23 <b>V</b> Vanadium 50.9415	24 <b>Cr</b> Chromium 51.9961	25 <b>Mn</b> Manganese 54.938044	26 <b>Fe</b> Iron 55.845	27 <b>Co</b> Cobalt 58.933194	28 <b>Ni</b> Nickel 58.6934	29 <b>Cu</b> Copper 63.546	30 <b>Zn</b> Zinc 65.38	31 <b>Ga</b> Gallium 69.723	32 <b>Ge</b> Germanium 72.630	33 <b>As</b> Arsenic 74.921595	34 <b>Se</b> Selenium 78.971	35 <b>Br</b> Bromine 79.904	36 <b>Kr</b> Krypton 83.798
37 <b>Rb</b> Rubidium 85.4678	38 <b>Sr</b> Strontium 87.62	39 <b>Y</b> Yttrium 88.90584	40 <b>Zr</b> Zirconium 91.224	41 <b>Nb</b> Niobium 92.90637	42 <b>Mo</b> Molybdenum 95.95	43 <b>Tc</b> Technetium (98)	44 <b>Ru</b> Ruthenium 101.07	45 <b>Rh</b> Rhodium 102.90550	46 <b>Pd</b> Palladium 106.42	47 <b>Ag</b> Silver 107.8682	48 <b>Cd</b> Cadmium 112.414	49 <b>In</b> Indium 114.818	50 <b>Sn</b> Tin 118.710	51 <b>Sb</b> Antimony 121.760	52 <b>Te</b> Tellurium 127.60	53 <b>I</b> Iodine 126.90447	54 <b>Xe</b> Xenon 131.293
55 <b>Cs</b> Caesium 132.90545196	56 <b>Ba</b> Barium 137.327	57 - 71 Lanthanoids	72 <b>Hf</b> Hafnium 178.49	73 <b>Ta</b> Tantalum 180.94788	74 <b>W</b> Tungsten 183.84	75 <b>Re</b> Rhenium 186.207	76 <b>Os</b> Osmium 190.23	77 <b>Ir</b> Iridium 192.217	78 <b>Pt</b> Platinum 195.084	79 <b>Au</b> Gold 196.966569	80 <b>Hg</b> Mercury 200.592	81 <b>Tl</b> Thallium 204.38	82 <b>Pb</b> Lead 207.2	83 <b>Bi</b> Bismuth 208.98040	84 <b>Po</b> Polonium (209)	85 <b>At</b> Astatine (210)	86 <b>Rn</b> Radon (222)
87 <b>Fr</b> Francium (223)	88 <b>Ra</b> Radium (226)	89 - 103 Actinoids	104 <b>Rf</b> Rutherfordium (267)	105 <b>Db</b> Dubnium (268)	106 <b>Sg</b> Seaborgium (269)	107 <b>Bh</b> Bohrium (270)	108 <b>Hs</b> Hassium (269)	109 <b>Mt</b> Meitnerium (278)	110 <b>Ds</b> Darmstadtium (281)	111 <b>Rg</b> Roentgenium (282)	112 <b>Cn</b> Copernicium (285)	113 <b>Nh</b> Nihonium (286)	114 <b>Fl</b> Flerovium (289)	115 <b>Mc</b> Moscovium (289)	116 <b>Lv</b> Livermorium (293)	117 <b>Ts</b> Tennesine (294)	118 <b>Og</b> Oganesson (294)

57 <b>La</b> Lanthanum 138.90547	58 <b>Ce</b> Cerium 140.116	59 <b>Pr</b> Praseodymium 140.90766	60 <b>Nd</b> Neodymium 144.242	61 <b>Pm</b> Promethium (145)	62 <b>Sm</b> Samarium 150.36	63 <b>Eu</b> Europium 151.964	64 <b>Gd</b> Gadolinium 157.25	65 <b>Tb</b> Terbium 158.92535	66 <b>Dy</b> Dysprosium 162.500	67 <b>Ho</b> Holmium 164.93033	68 <b>Er</b> Erbium 167.259	69 <b>Tm</b> Thulium 168.93422	70 <b>Yb</b> Ytterbium 173.045	71 <b>Lu</b> Lutetium 174.9668
89 <b>Ac</b> Actinium (227)	90 <b>Th</b> Thorium 232.0377	91 <b>Pa</b> Protactinium 231.03588	92 <b>U</b> Uranium 238.02891	93 <b>Np</b> Neptunium (237)	94 <b>Pu</b> Plutonium (244)	95 <b>Am</b> Americium (243)	96 <b>Cm</b> Curium (247)	97 <b>Bk</b> Berkelium (247)	98 <b>Cf</b> Californium (251)	99 <b>Es</b> Einsteinium (252)	100 <b>Fm</b> Fermium (257)	101 <b>Md</b> Mendelevium (258)	102 <b>No</b> Nobelium (259)	103 <b>Lr</b> Lawrencium (260)

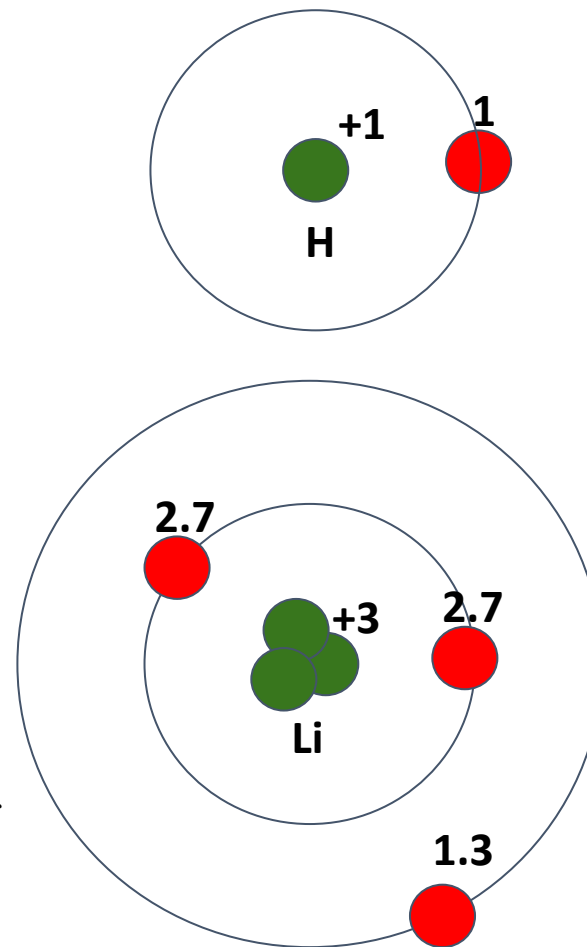
# Effective nuclear charge : Slater's rule

In a multi-electronic system, **effective nuclear charge** ( $Z_{\text{eff}}$ ) is the amount of net charge experienced by any individual electron, which is always less than actual nuclear charge ( $Z$ ).

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

$\sigma$  = shielding constant

$Z_{\text{eff}}$  depends on distance from the nucleus.  
Closer electrons feel comparatively higher  $Z_{\text{eff}}$  than distant electrons.



# Rules for calculation of $\sigma$

## **Electrons in same group:**

Each other electron in the same group, i.e., ns, np, nd or nf-electrons contribute 0.35 to  $\sigma$  (except 1s-electron for which  $\sigma=0.3$ ).

## **Electrons in lower group:**

For s or p subshell, all electrons in next lower shell (n - 1) contribute 0.85 and all electrons in even lower shells (n-2) contribute 1.0 to  $\sigma$ .

For nd or nf subshell, every electron in groups to the lower contributes 1.0 to  $\sigma$ .

• **Exercise:** Calculate  $Z_{\text{eff}}$  for  $\text{Na}^+$ .

**Qn.** Calculate the effective nuclear charge for (i) 3p electron in Sulphur,  
(ii) 4s electron in K?

**Ans:** (i) S (16) =  $1s^2 2s^2 2p^6 3s^2 3p^4$

$$\begin{aligned}\sigma &= (5 \times 0.35) + (8 \times 0.85) + (2 \times 1) \\ &= 10.55\end{aligned}$$

$$\begin{aligned}Z_{\text{eff}} &= Z - \sigma \\ &= 16 - 10.55 \\ &= 5.45\end{aligned}$$

(ii) K (19) =  $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$

$$\begin{aligned}\text{For } 4s^1, \sigma &= (8 \times 0.85) + (10 \times 1) \\ &= 16.8\end{aligned}$$

$$\begin{aligned}Z_{\text{eff}} &= Z - \sigma \\ &= 19 - 16.8 \\ &= 2.2\end{aligned}$$

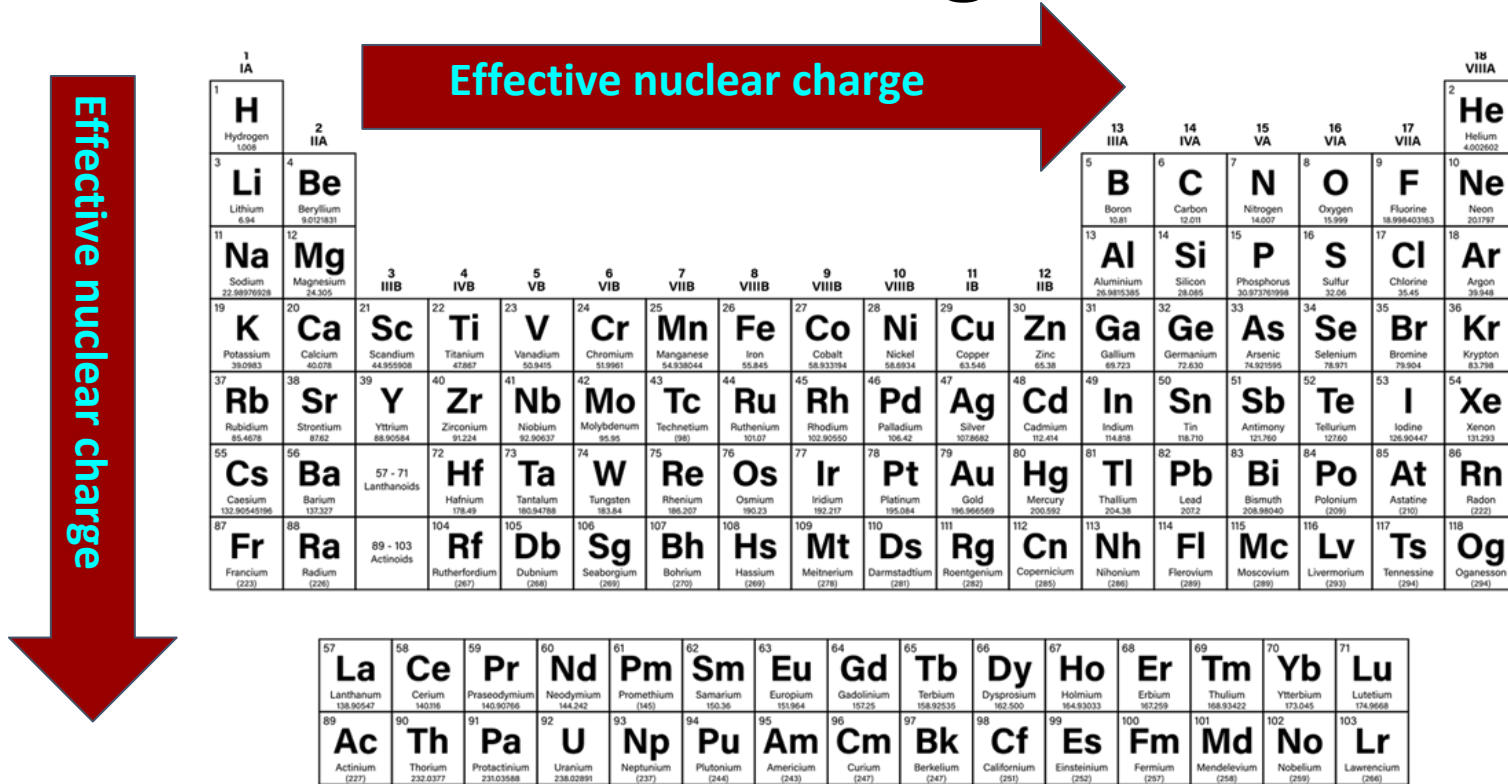
For F<sup>-</sup> ion:  $1s^2 2s^2 2p^6$

$$\begin{aligned}\sigma &= 7 \times 0.35 + 2 \times 0.85 \\ &= 2.45 + 1.70 \\ &= 4.15\end{aligned}$$

$$\begin{aligned}\text{Effective nuclear charge} &= 9 - 4.15 \\ &= 4.85\end{aligned}$$



# Periodic trends : Effective nuclear charge



**Effective nuclear charge**

1 IA	2 IIA											13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
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# Penetration of orbital

**Penetration of orbital** is defined as the proximity to which an electron can come near the nucleus.

In a multi-electronic system, it is measured by the relative density of electrons (probability density) close to the nucleus.

If shell value (n) is same, then the penetration of an electron follows the following trend in subshells ( $m_l$ ):

$$s > p > d > f$$

For different values of shell and subshell, it follows the trend:

$$1s > 2s > 2p > 3s > 3p > 4s > 3d > 4p > 5s > 4d > 5p > 6s > 4f \dots$$

which is also the exact reverse trend for the energy of the electrons.

## Variations of s, p, d and f orbital energies in the periodic table

### For single-electron system (H, He<sup>+</sup>):

- ❑ Ground state has the least energy than the excited states.
- ❑ The energy is decided by the principal quantum number
- ❑ If the principal quantum number ( $n$ ) is same, then all the the orbitals become degenerate.

### For multi-electron system:

- ❑ The energy is decided by the principal quantum number as well as the azimuthal quantum number ( $n + l$ ).
- ❑ If ( $n + l$ ) is same then higher  $n$  has higher energy value.
- ❑ Orbitals experiencing higher shielding effect has higher energy.

Exercise: 3d and 4s which has the higher energy and why?  
4p and 5s which has the higher energy and why?

# Periodic properties : Electronic configurations

Electrons occupy the orbitals following these 3 principles,

## Aufbau principle:

Electrons fill in the orbitals following the order of increasing energy, which means the lowest energy orbitals are occupied first and then the higher energy orbitals.

1s---2s---2p---3s---3p---4s---3d---4p---5s---4d---5p---6s---4f

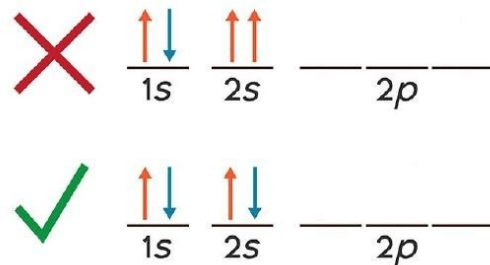
## Hund's rule:

Pairing of electrons are possible only when all other degenerate orbitals are singly occupied.

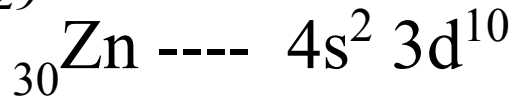
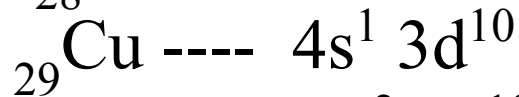
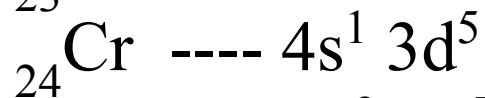
# Electronic configurations

## Pauli's exclusion principle:

In an atom or molecule, **no two electrons can have all 4 quantum numbers same.**



Consider the following pairs



# Atomic and ionic radius

- ❖ For metals (Left hand side of the periodic table, for example Group I, II, IIIA), they lose electron to become +ve cations, and the size of their cation always decreases as the outermost shell is emptied after electron donation.
- ❖ Moreover, in cation the number of proton is higher than the number of electron as compared to neutral atom, as a result nuclear attraction is more effective.
- ❖ Along the period, the atomic and cationic sizes decrease as a result of increasing effective nuclear charge as well as higher number of protons compared to electrons in the cations.
- ❖ Across the group, the atomic and cationic sizes increase simply because more shells are added gradually.

# Atomic and ionic radius

- ❑ For nonmetals (right hand side of the periodic table, Group V, VI, VIIA), they accept electron to become -ve anions, and the size of their anion always increases as in the outermost shell interelectronic repulsion increases.
- ❑ Moreover, in anion the number of proton is lower than the number of electron as compared to neutral atom, as a result nuclear attraction become less effective.
- ❑ Along the period, the atomic and anionic sizes decreases as a result of increasing effective nuclear charge as well as decreasing charge of the stable anions.
- ❑ Across the group, the the atomic and anionic sizes increases simply because more shells are added gradually.

# Periodic trends : Atomic radius

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# Sizes of atoms and their ions in pm




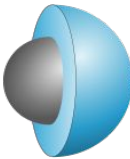
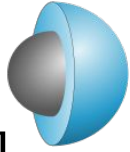


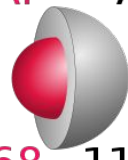
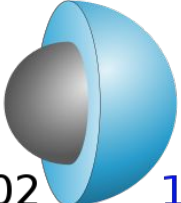
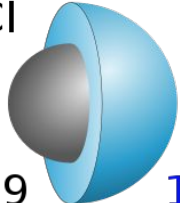
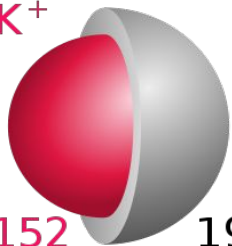
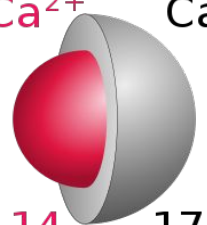
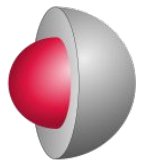
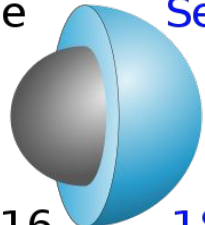
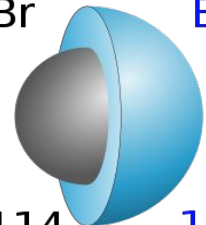
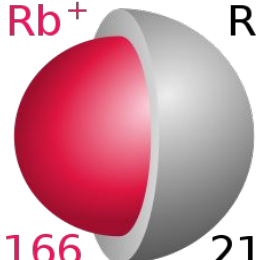
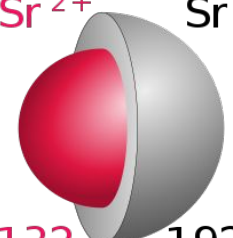
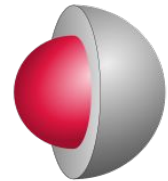
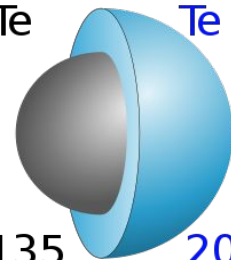
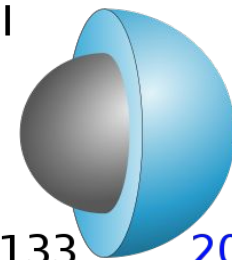
Group 1

Group 2

Group 13

Group 16

Group 17

$\text{Li}^+$  90 Li 134	$\text{Be}^{2+}$  59 Be 90	$\text{B}^{3+}$  41 B 82	O  73 $\text{O}^{2-}$ 126	F  71 $\text{F}^-$ 119
$\text{Na}^+$  116 Na 154	$\text{Mg}^{2+}$  86 Mg 130	$\text{Al}^{3+}$  68 Al 118	S  102 $\text{S}^{2-}$ 170	Cl  99 $\text{Cl}^-$ 167
$\text{K}^+$  152 K 196	$\text{Ca}^{2+}$  114 Ca 174	$\text{Ga}^{3+}$  76 Ga 126	Se  116 $\text{Se}^{2-}$ 184	Br  114 $\text{Br}^-$ 182
$\text{Rb}^+$  166 Rb 211	$\text{Sr}^{2+}$  132 Sr 192	$\text{In}^{3+}$  94 In 144	Te  135 $\text{Te}^{2-}$ 207	I  133 $\text{I}^-$ 206

# Ionization energy

The quantity of energy required to remove an electron from an atom is called as the **ionization energy**.

Ionization energy is usually expressed in terms of electron volt (eV) per atom or kJ/mole.

$$1 \text{ eV/atom} = 96.48 \text{ kJ/mol}$$

**Low IE: Easy to remove an electron from the atom**

**High IE: Hard to remove an electron from the atom**

**Factors affecting the ionization energy**

## ❖ **Effective nuclear charge**

- Higher the effective nuclear charge, higher the force of attraction between the nucleus and the electron and hence higher the ionization energy

## ❖ **Size of the atom**

- With the increase in the size of the atom, the electrons remain farther from the nucleus. As a result, the force of attraction between the nucleus and the outermost electron decreases and the ionization energy

# Trend in Ionization energy

**What happens down a group?**

**The ionization energy decreases down the group.**

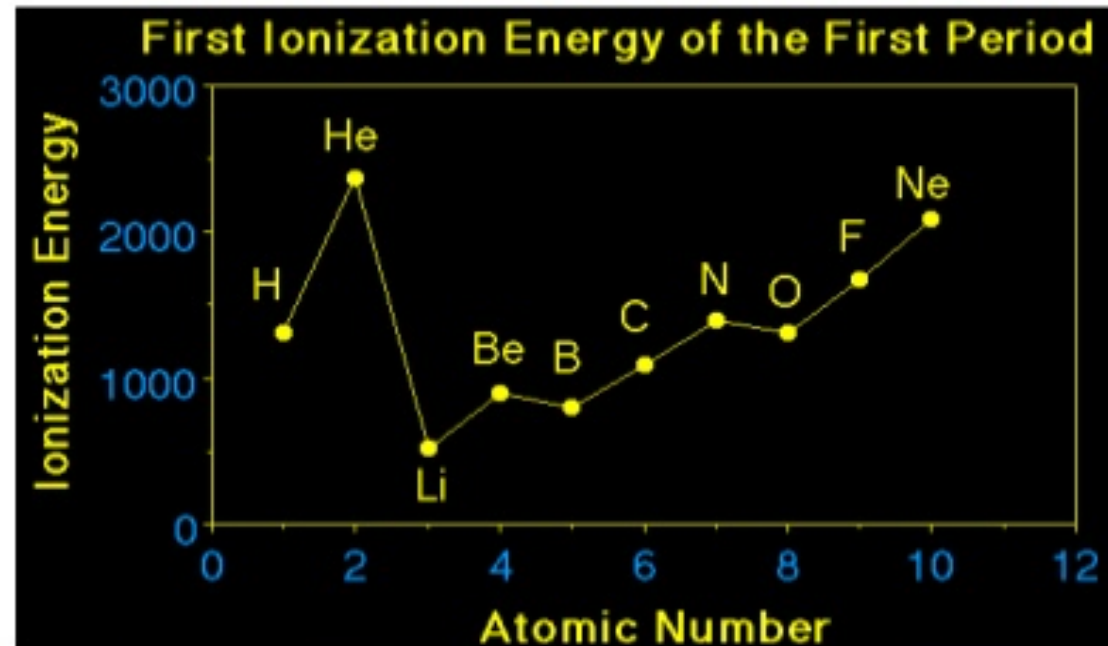
As the size of atom increases down the group, the attraction becomes weaker between the outer shell electrons and the nucleus. Hence less energy is required to remove an electron from the outermost shell.

**What happens across a period?**

**The ionization energy increases along a period.**

Across a period, as the size of atom decreases from left to right, the force of attraction between the nucleus and electrons increases. Hence higher energy is required to remove the electron from the outermost shell.

- As the period begins it does not take a lot of energy to remove an electron from Li but as you go across the period it takes more and more energy to take an electron away



# Electron Affinity

The amount of energy released when an electron is added to a neutral atom in gaseous state is called as its electron affinity.



## Factors affecting the electron affinity

### ❖ Effective nuclear charge

- Higher the effective nuclear charge of the atom, higher the force of attraction between the nucleus and the additional electron and hence higher the electron affinity

### ❖ Size of the atom

- Smaller the size of the atom, smaller will be the distance between the nucleus and the additional electron. As a result, the force of attraction between the nucleus and the outermost electron increases and the electron affinity increases with the smaller size of the atom.

## ❖ **Electronic configuration**

Atoms having stable electronic configuration (half-filled or full-filled outer orbitals) do not show much tendency for an extra electron. Hence they have either zero or very low electron affinity.

# Trend in Electron Affinity

**What happens down a group?**

**The electron affinity decreases down the group.**

As the size of atom increases down the group, the attraction becomes weaker between the nucleus of atom and the additional electron.

Hence the atom possess less electron affinity.

**What happens across a period?**

**The electron affinity increases on moving from left to right along a period.**

Across a period, as the size of atom decreases from left to right, the force of attraction between the nucleus and electrons increases.

Hence the electron affinity increases along the period from left to right.

# Electronegativity

The ability of an atom to attract the shared electrons towards itself is called as its electronegativity.

**Note:** Electronegativity is not a property of an atom alone, but rather a property of an atom in a **molecule**

- ❖ The term "electronegativity" was introduced by Jöns Jacob Berzelius in 1811.
- ❖ An accurate scale of electronegativity was not developed until 1932, when **Linus Pauling** proposed an electronegativity scale
- ❖ Electronegativity cannot be directly measured and must be calculated from other atomic or molecular properties.



## Pauling electronegativity:

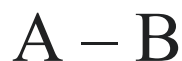
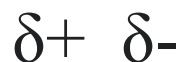
Let us consider the formation of A-B from A<sub>2</sub> and B<sub>2</sub>



The molecular orbital for AB is:

$$\phi_{\text{AB}} = \psi_{\text{A}} + c (\psi_{\text{B}})$$

If  $c > 1$ , then the molecular orbital is concentrated on atom B, which will acquire a partial negative charge.



The difference in electronegativity between atoms A and B is given by

$$|\chi_{\text{A}} - \chi_{\text{B}}| = (\text{eV})^{-1/2} [E_{\text{d}}(\text{AB}) - (E_{\text{d}}(\text{AA}) + E_{\text{d}}(\text{BB}))/2]^{1/2}$$

where  $E_{\text{d}}$  represents the bond dissociation energy in eV

## Mulliken electronegativity:

Robert S. Mulliken proposed that the arithmetic mean of the first **ionization energy** ( $E_i$ ) and the **electron affinity** ( $E_{ea}$ ) should be a measure of the tendency of an atom to attract electrons.

$$\chi = (E_i + E_{ea})/2 \text{ (in eV)}$$

# Trend in Electronegativity

In general, electronegativity increases on passing from left to right along a period and decreases on descending a group.

Hence, fluorine is the most electronegative of the elements, whereas Francium is the least electronegative.

## Electronegativity

Electronegativity																					
1		2												3	4	5	6	7	8		
														(13)	(14)	(15)	(16)	(17)	(18)		