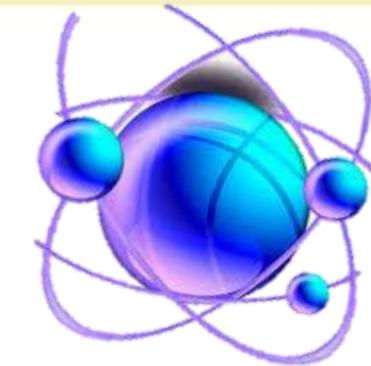




MS31007: Materials Science

Chapter 2

Atomic Structure and Bonding



- Interatomic Bonding
- Bonding forces and energies
- Primary interatomic bonds
- Secondary bonding
- Molecules

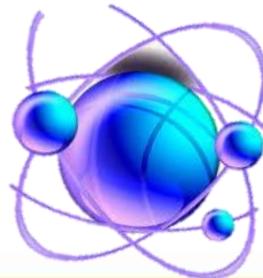
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Chapter 2: Atomic Structure and Bonding

Learning Objectives

- Define four **quantum numbers** for electrons and explain the significance of each.
- Explain the arrangement of the elements in the **periodic table**.
- State the **electronic structure** of the elements.
- Explain the role of **electronegativity in bonding**.
- Define four different **mechanisms of bonding** in materials.
- Understand how **interactions between atoms or between ions** influence materials properties.
- Recognize that even though **allotropes** are composed of the same element, they can display dramatically different materials properties based on their structure (e.g., the allotropes of carbon).





Nature of Interatomic Bonding

Why the individual atoms coalesce into larger structures and take on the characteristics and properties of many different materials?

The bonding mechanisms between atoms are closely related to the structure of the atoms themselves.

Atoms = nucleus (protons and neutrons) + electrons

Charges: Electrons and protons have negative and positive charges of the same magnitude, 1.6×10^{-19} Coulombs.

Neutrons are electrically neutral.

Masses: Protons and Neutrons have the same mass, 1.67×10^{-27} kg.

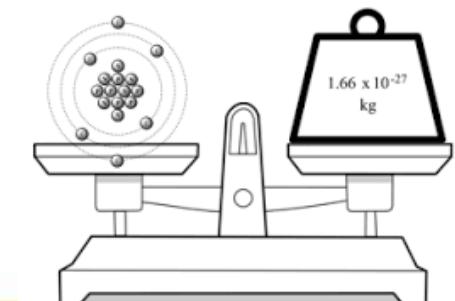
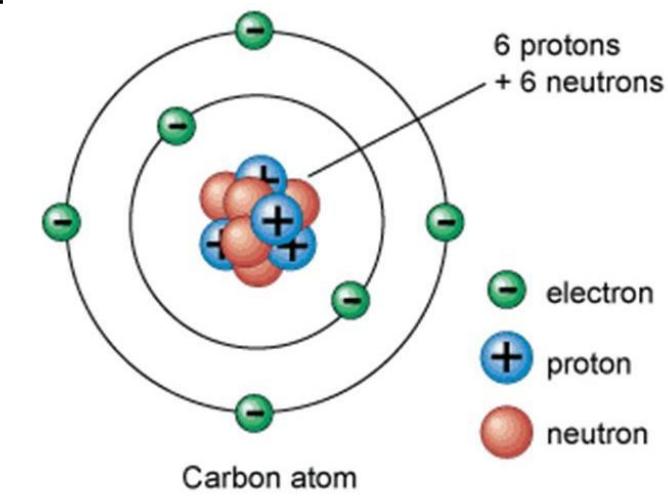
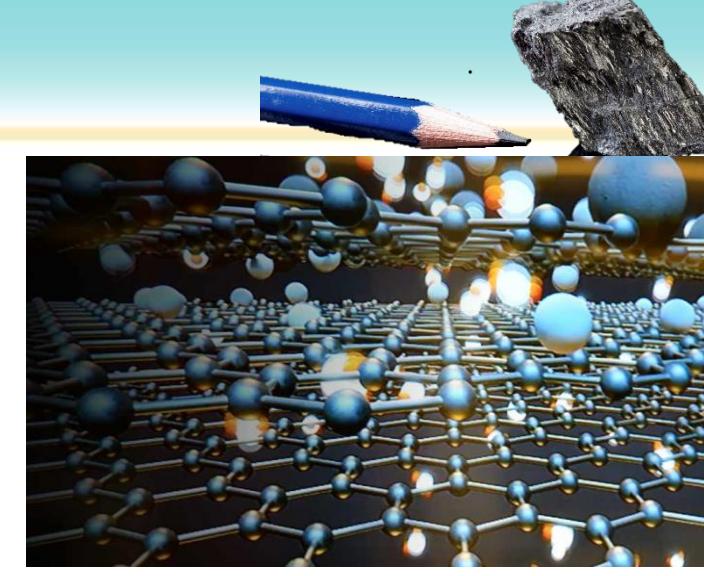
Mass of an electron is much smaller, 9.11×10^{-31} kg and can be neglected in calculation of atomic mass.

The atomic mass (A) = mass of Protons + mass of Neutrons

protons gives chemical identification of the element

protons = atomic number (Z)

neutrons defines isotope number





Atomic mass units. Atomic weight

The atomic mass unit (**amu**) is often used to express **atomic weight**.

1 amu is defined as 1/12 of the atomic mass of the most common isotope of carbon atom that has 6 protons ($Z=6$) and six neutrons ($N=6$).

$$M_{\text{proton}} \approx M_{\text{neutron}} = 1.66 \times 10^{-24} \text{ g} = 1 \text{ amu}$$

The atomic mass of the ^{12}C atom is 12 amu.

The atomic weight of an element = weighted average of the atomic masses of the atoms naturally occurring isotopes. Atomic weight of carbon is 12.011 amu. The atomic weight is often specified in mass per mole.

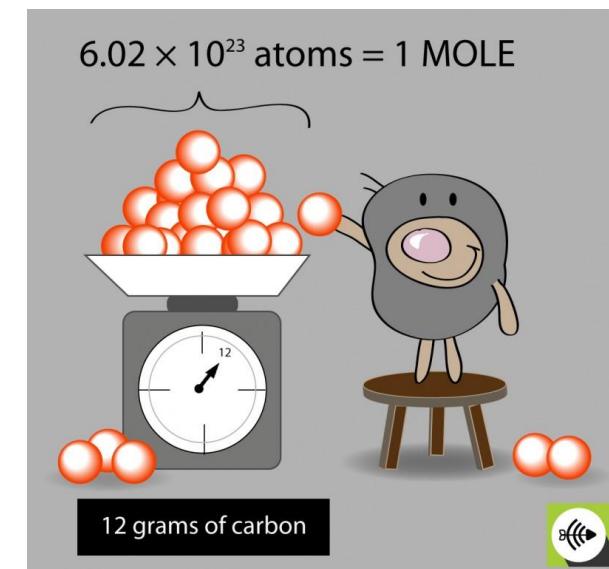
A **mole** is the amount of matter that has a mass in grams equal to the atomic mass in **amu** of the atoms (A mole of carbon has a mass of 12 grams).

The number of atoms in a mole =

$$\text{Avogadro number}, N_{\text{av}} = 6.023 \times 10^{23}$$

$$1 \text{ amu/atom} = 1 \text{ gram/mol}$$

Example: Atomic weight of iron (Fe) = 55.85 amu/atom
= 55.85 g/mol





Some simple calculations

The number of atoms per cm^3 , n , for material of density $d(\text{g}/\text{cm}^3)$ and atomic mass $M (\text{g/mol})$:

$$n = N_{av} \times d / M$$

Graphite (carbon): $d = 2.3 \text{ g}/\text{cm}^3$, $M = 12 \text{ g/mol}$,
 $n = 6 \times 10^{23} \text{ atoms/mol} \times 2.3 \text{ g}/\text{cm}^3 / 12 \text{ g/mol} = 11.5 \times 10^{22} \text{ atoms}/\text{cm}^3$

Diamond (carbon): $d = 3.5 \text{ g}/\text{cm}^3$, $M = 12 \text{ g/mol}$
 $n = 6 \times 10^{23} \text{ atoms/mol} \times 3.5 \text{ g}/\text{cm}^3 / 12 \text{ g/mol} = 17.5 \times 10^{22} \text{ atoms}/\text{cm}^3$

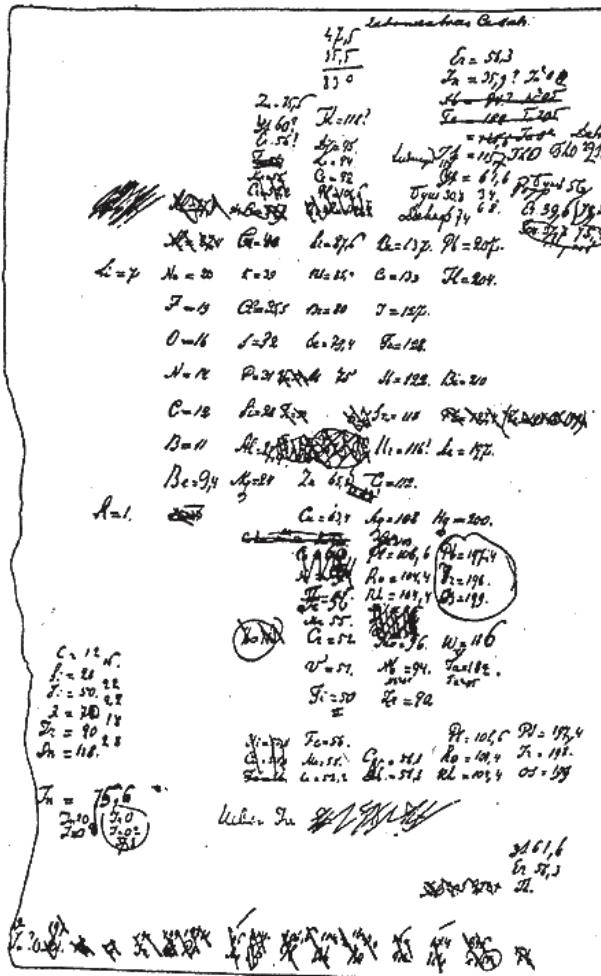
For material with $n = 6 \times 10^{22} \text{ atoms}/\text{cm}^3$ we can calculate
mean distance between atoms $L = (1/n)^{1/3} = 0.25 \text{ nm}$.

Water (H_2O) $d = 1 \text{ g}/\text{cm}^3$, $M = 18 \text{ g/mol}$
 $n = 6 \times 10^{23} \text{ molecules/mol} \times 1 \text{ g}/\text{cm}^3 / 18 \text{ g/mol}$
 $= 3.3 \times 10^{22} \text{ molecules}/\text{cm}^3$



Periodic Table

The first accepted periodic table of elements was published in **1869 by Mendeleev**. In the same year, a German chemist Lothar Meyer independently published a very similar table, but his contribution is generally ignored.



All elements in the periodic table have been classified according to the electron configuration.

Draft of the periodic table,
Mendeleev, 1869



Periodic Table of the Elements

Arranged by
**atomic
number,**
**electron
configuration**
**& recurring
chemical
properties**

Periodic Table of the Elements																						
Group 1		Period 18																				
1	la																					
1	H	1.01	2	IIa																		
	Hydrogen 1s ¹			Beryllium 1s ² s ²																		
2	Li	6.94	4	Be	9.01																	
	Lithium 1s ² s ¹			Beryllium 1s ² s ²																		
3	Na	22.99	12	Mg	24.31	3	4	5	6	7	8	9	10	11	12	13	14					
	Sodium [Ne]3s ¹			Magnesium [Ne]3s ²		IIIb	IVb	Vb	VIb	VIIb	VIIIb	←	→	Ib	IIb	IIIa	IVa					
4	K	39.10	20	Ca	40.08	21	44.96	22	Ti	47.87	23	50.94	24	52.00	25	54.94	26	55.85				
	Potassium [Ar]4s ¹			Calcium [Ar]4s ²		Scandium [Ar]3d ¹ 4s ²	Titanium [Ar]3d ² 4s ²	Vanadium [Ar]3d ³ 4s ²	Chromium [Ar]3d ⁴ 4s ¹	Manganese [Ar]3d ⁵ 4s ²	Iron [Ar]3d ⁶ 4s ²	Cobalt [Ar]3d ⁷ 4s ²	Nickel [Ar]3d ⁸ 4s ²	Copper [Ar]3d ⁹ 4s ¹	Zinc [Ar]3d ¹⁰ 4s ²	Aluminum [Ne]3s ² p ¹	Boron [Ne]3s ² p ¹	Carbon [Ne]3s ² p ²	Nitrogen [Ne]3s ² p ³	Oxygen [Ne]3s ² p ⁴	Fluorine [Ne]3s ² p ⁵	Neon [Ne]3s ² p ⁶
5	Rb	85.47	38	Sr	87.62	39	88.91	40	Zr	91.22	41	92.91	42	95.94	43	(98)	44	101.07				
	Rubidium [Kr]5s ¹			Strontium [Kr]5s ²		Yttrium [Kr]4d ¹ 5s ²	Zirconium [Kr]4d ² 5s ²	Niobium [Kr]4d ³ 5s ¹	Molybdenum [Kr]4d ⁴ 5s ¹	Technetium [Kr]4d ⁵ 5s ²	Ruthenium [Kr]4d ⁶ 5s ¹	Rhodium [Kr]4d ⁷ 5s ¹	Palladium [Kr]4d ⁸ 5s ¹	Silver [Kr]4d ⁹ 5s ¹	Cadmium [Kr]4d ¹⁰ 5s ²	Gallium [Ar]3d ¹⁰ 4s ² p ¹	Germanium [Ar]3d ¹⁰ 4s ² p ²	Arsenic [Ar]3d ¹⁰ 4s ² p ³	Selenium [Ar]3d ¹⁰ 4s ² p ⁴	Bromine [Ar]3d ¹⁰ 4s ² p ⁵	Krypton [Ar]3d ¹⁰ 4s ² p ⁶	
6	Cs	132.91	56	Ba	137.33		72	178.49	73	Ta	180.95	74	183.84	75	186.21	76	190.23					
	Cesium [Xe]6s ¹			Barium [Xe]6s ²		◆	Hafnium [Xe]4f ¹ 5d ² 6s ²	Tantalum [Xe]4f ¹ 5d ³ 6s ²	Tungsten [Xe]4f ¹ 5d ⁴ 6s ²	Rhenium [Xe]4f ¹ 5d ⁵ 6s ²	Osmium [Xe]4f ¹ 5d ⁶ 6s ²	Iridium [Xe]4f ¹ 5d ⁷ 6s ²	Platinum [Xe]4f ¹ 5d ⁸ 6s ¹	Gold [Xe]4f ¹ 5d ⁹ 6s ¹	Mercury [Xe]4f ¹ 5d ¹⁰ 6s ¹	Thallium [Xe]4f ¹ 5d ¹¹ 6s ² p ¹	Lead [Xe]4f ¹ 5d ¹¹ 6s ² p ²	Bismuth [Xe]4f ¹ 5d ¹¹ 6s ² p ³	Polonium [Xe]4f ¹ 5d ¹¹ 6s ² p ⁴	Astatine [Xe]4f ¹ 5d ¹¹ 6s ² p ⁵	Radon [Xe]4f ¹ 5d ¹¹ 6s ² p ⁶	
7	Fr	(223)	88	(226)			104	(265)	105	(268)	106	(271)	107	(270)	108	(277)	109	(276)				
	Francium [Rn]7s ¹			Rutherfordium [Rn]5f ¹ 6d ⁵ 7s ²			Dubnium [Rn]5f ¹ 6d ⁷ 7s ²	Seaborgium [Rn]5f ¹ 6d ⁷ 7s ²	Bohrium [Rn]5f ¹ 6d ⁷ 7s ²	Hassium [Rn]5f ¹ 6d ⁷ 7s ²	Meitnerium [Rn]5f ¹ 6d ⁷ 7s ¹	Darmstadtium [Rn]5f ¹ 6d ⁷ 7s ¹	Roentgenium [Rn]5f ¹ 6d ⁷ 7s ¹	Copernicium [Rn]5f ¹ 6d ⁷ 7s ¹	Ununtrium [Rn]5f ¹ 6d ⁷ 7s ¹	Flerovium [Rn]5f ¹ 6d ⁷ 7s ¹	Ununpentium [Rn]5f ¹ 6d ⁷ 7s ¹	Livermorium [Rn]5f ¹ 6d ⁷ 7s ¹	Ununseptium [Rn]5f ¹ 6d ⁷ 7s ¹	Ununoctium [Rn]5f ¹ 6d ⁷ 7s ¹		

Aa -Solid



Aa -Gas

Aa -Liquids

Aa - Synthetically Prepared

57	138.91	58	140.12	59	140.91	60	144.24	61	(145)	62	150.36	63	151.96	64	157.25	65	158.93	66	162.50	67	164.93	68	167.26	69	168.93	70	173.04	71	174.9
La	Cerium	Ce	Praseodymium	Pr	Neodymium	Nd	Promethium	Pm	Samarium	Sm	Europium	Eu	Gadolinium	Gd	Terbium	Tb	Dysprosium	Dy	Holmium	Ho	Erbium	Er	Thulium	Tm	Ytterbium	Yb	Lutetium	Lu	
Lanthanum [Xe]5d ¹ 6s ²	Cerium [Xe]4f ¹ 5d ¹ 6s ²		Praseodymium [Xe]4f ⁶ s ²		Neodymium [Xe]4f ⁹ s ²		Promethium [Xe]4f ¹⁰ s ²		Samarium [Xe]4f ⁹ s ²		Europium [Xe]4f ⁷ s ²		Gadolinium [Xe]4f ⁵ 5d ¹ 6s ²		Terbium [Xe]4f ⁹ 6s ²		Dysprosium [Xe]4f ¹⁰ 6s ²		Holmium [Xe]4f ¹¹ 6s ²		Erbium [Xe]4f ¹² 6s ²		Thulium [Xe]4f ¹³ 6s ²		Ytterbium [Xe]4f ¹⁴ 5d ¹ 6s ²		Lutetium [Xe]4f ¹⁴ 5d ¹ 6s ²		
89	(227)	90	232.04	91	231.04	92	238.03	93	(237)	94	(244)	95	(243)	96	(247)	97	(247)	98	(251)	99	(252)	100	(257)	101	(258)	102	(259)	103	(262)
Ac	Thorium	Th	Protactinium	Pa	Uranium	U	Neptunium	Np	Plutonium	Pu	Americium	Am	Curium	Cm	Berkelium	Bk	Cf	Cf	Es	Es	Fm	Fm	Md	Md	No	No	Lr	Lr	
Actinium [Rn]5d ¹ 7s ²	Thorium [Rn]4f ¹ 5d ¹ 7s ²		Protactinium [Rn]5f ⁵ 6d ¹ 7s ²		Uranium [Rn]5f ⁷ 6d ¹ 7s ²		Neptunium [Rn]5f ⁹ 6d ¹ 7s ²		Plutonium [Rn]5f ¹¹ 6d ¹ 7s ²		Americium [Rn]5f ¹³ 7s ²		Curium [Rn]5f ¹⁵ 7s ²		Berkelium [Rn]5f ¹⁷ 7s ²		Californium [Rn]5f ¹⁹ 7s ²		Einsteinium [Rn]5f ²¹ 7s ²		Fermium [Rn]5f ²³ 7s ²		Mendelevium [Rn]5f ²⁵ 7s ²		Nobelium [Rn]5f ²⁷ 7s ²		Lawrencium [Rn]5f ²⁷ 7s ²		



Electrons in Atoms

The electrons form a cloud around the nucleus, of radius of 0.05 – 2 nm.

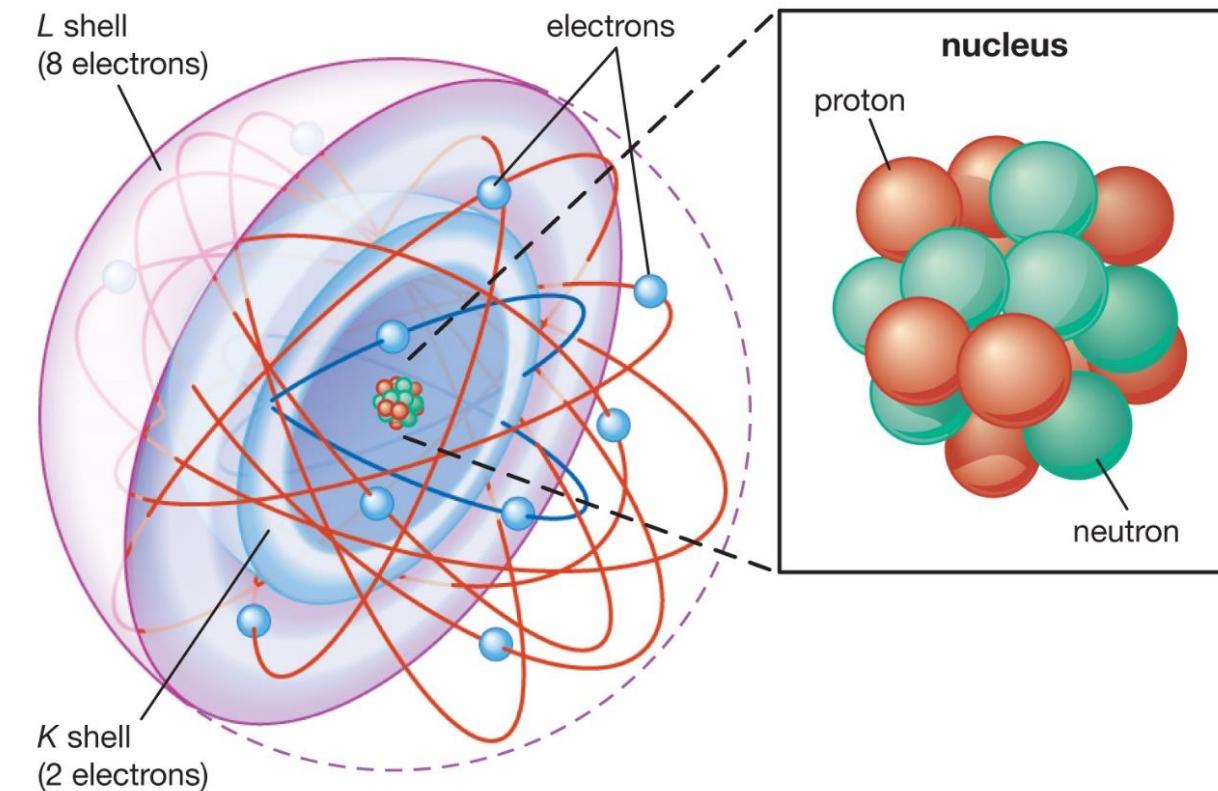
Only certain “orbits” or shells of electron probability densities are allowed

The shells are identified by a **principal quantum number n**, which can be related to the size of the shell, $n = 1$ is the smallest;

$n = 2, 3 \dots$ are larger.

The second quantum number l, defines subshells within each shell.

Two more quantum numbers characterize states within the subshells.

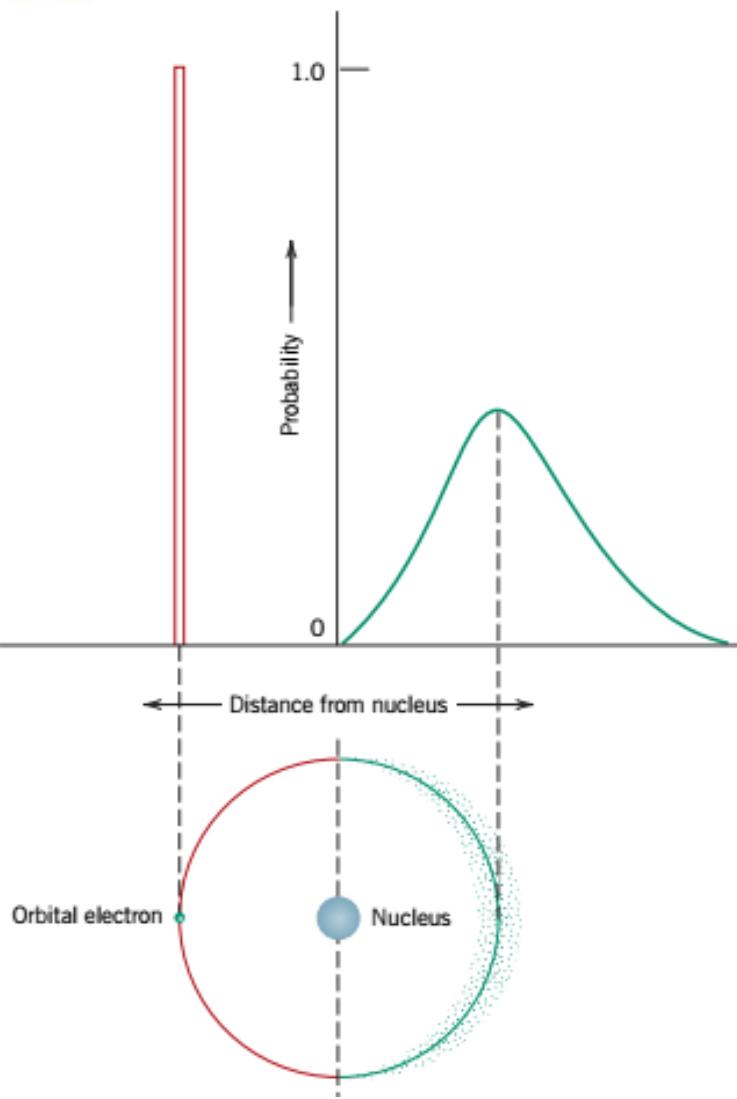


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Pauli Exclusion Principle: only one electron can have a given set of the four Quantum numbers.



Quantum Numbers



Comparison of the (a) Bohr and (b) wave mechanical atom models in terms of electron distribution

The quantum numbers arise from solution of Schrodinger's equation

$$\frac{-\hbar^2}{2m} \nabla^2 \Psi(r) + V(r)\Psi(r) = E\Psi(r)$$

$$\text{Kinetic Energy} + \text{Potential Energy} = \text{Total Energy}$$

Eigenvalues are discrete energy levels for electron

Square of eigenfunction gives probability density (where electron can be found)

$$E_n = -\frac{me^4}{32\pi^2 \epsilon_0^2 \hbar^2} \left(\frac{1}{n^2}\right)$$

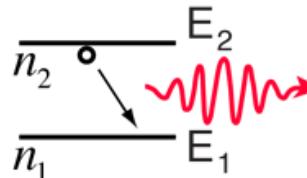
$$\Psi_{1,0,0} = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

a_0 = Bohr radius



Electrons in Hydrogen Atoms

The Bohr model for an electron transition in H between quantized energy levels with different quantum numbers ***n*** yields a photon by emission with quantum energy:

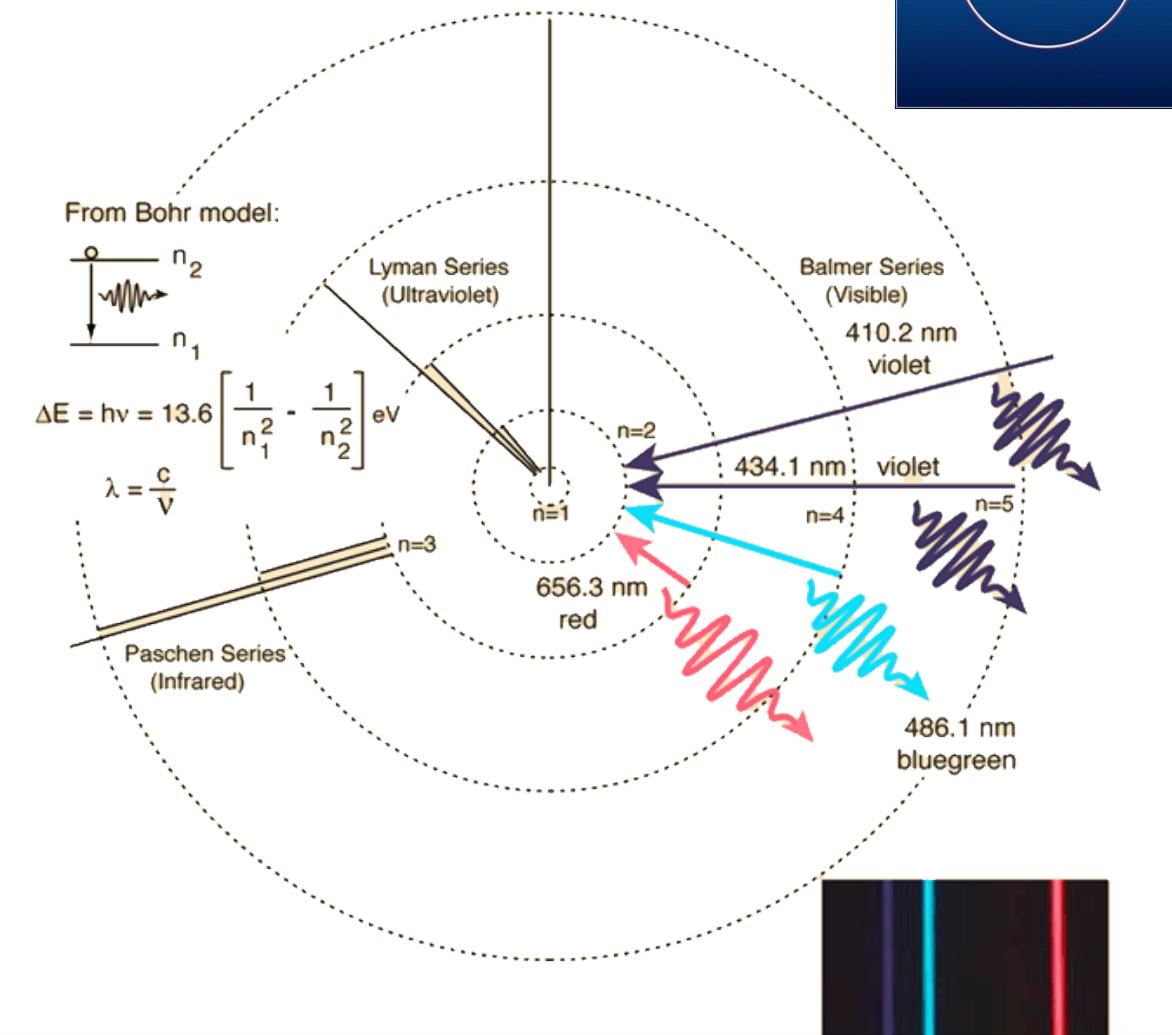
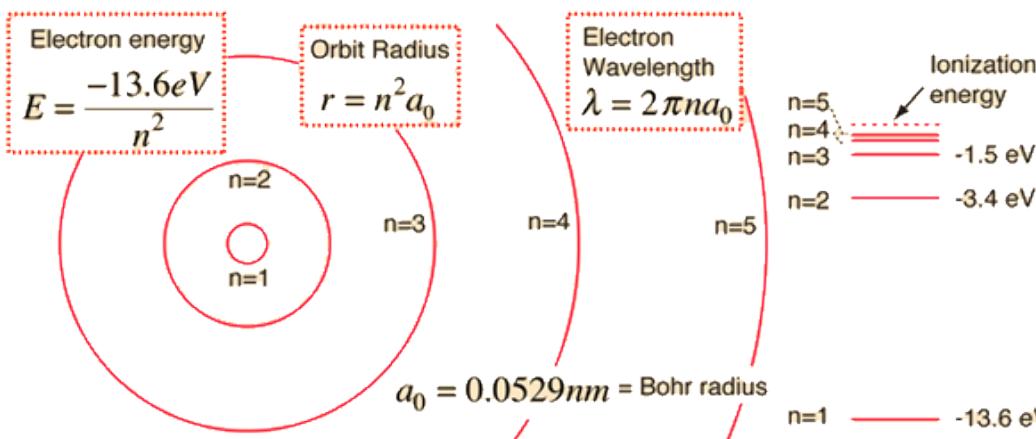


A downward transition involves emission of a photon of energy:

$$E_{\text{photon}} = h\nu = E_2 - E_1$$

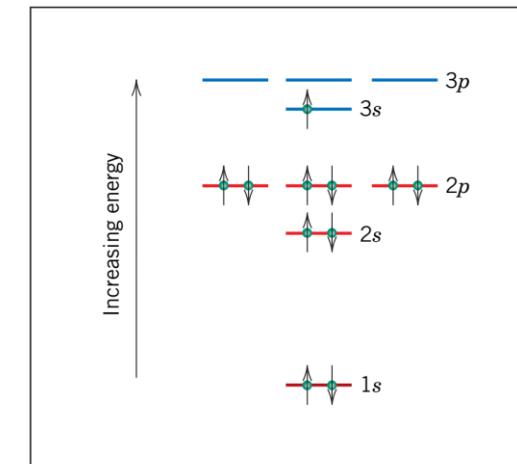
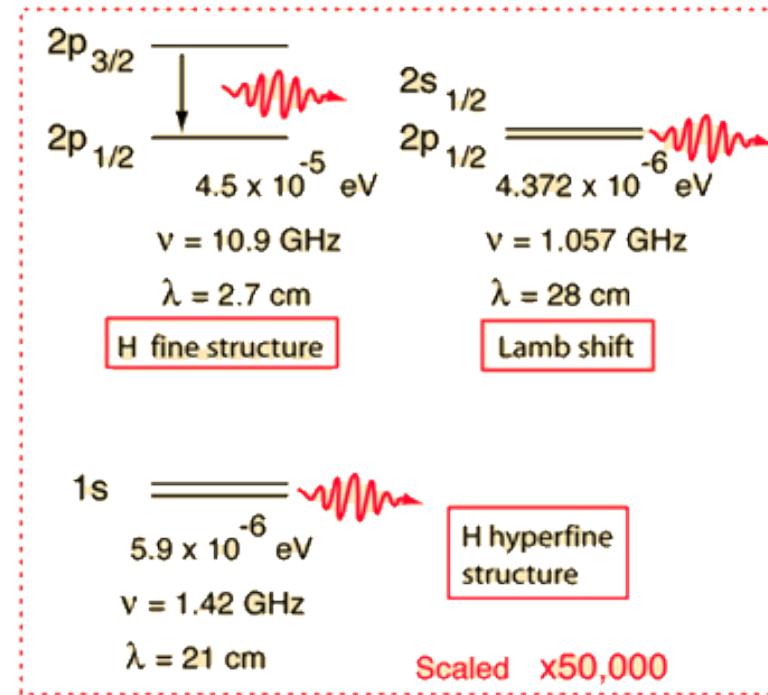
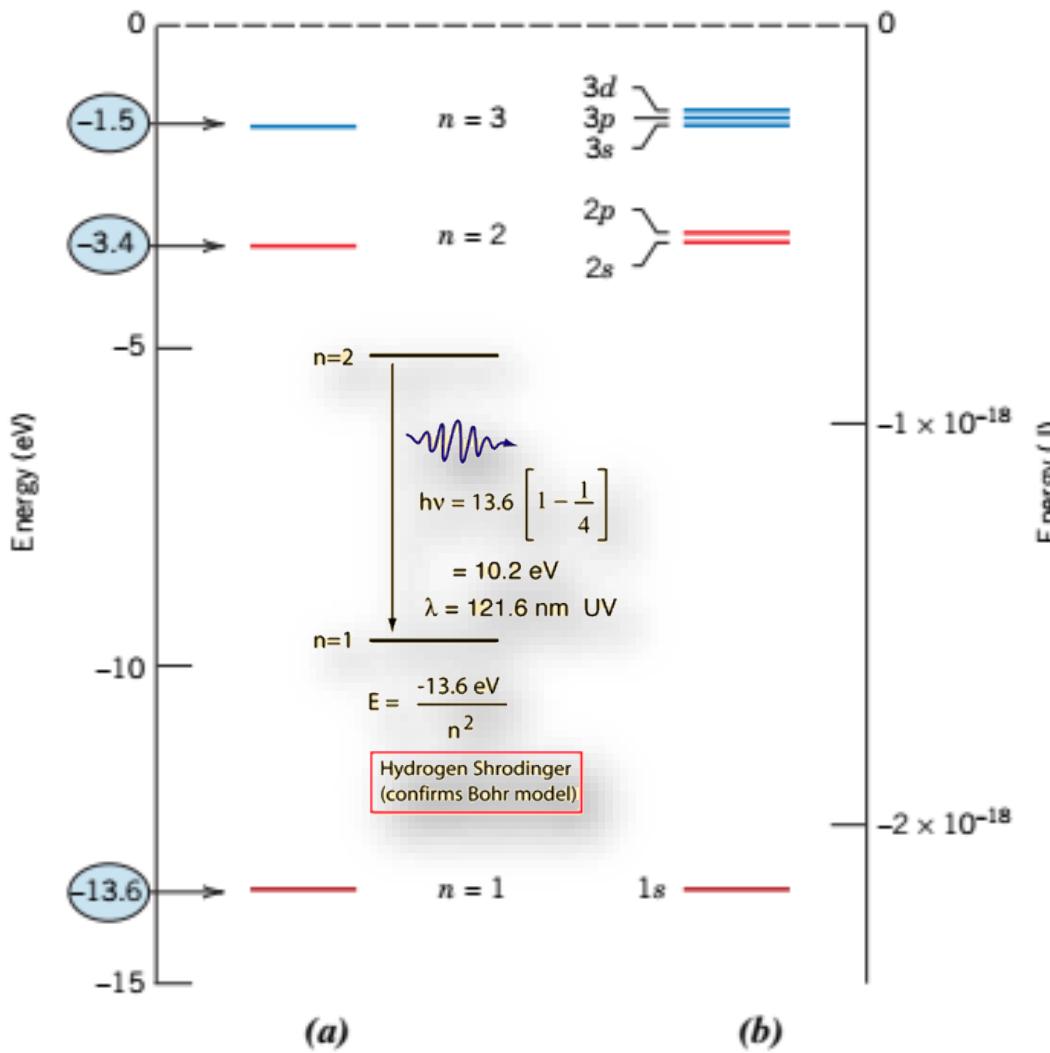
Given the expression for the energies of the hydrogenic electron states for atoms of atomic number Z:

$$h\nu = \frac{Z^2 me^4}{8h^2 \epsilon_0^2} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] = -13.6Z^2 \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \text{ eV}$$





Electrons in Hydrogen Atoms



- (a) The first three electron energy states for the Bohr hydrogen atom.
- (b) Electron energy states for the first three shells of the wave-mechanical hydrogen atom

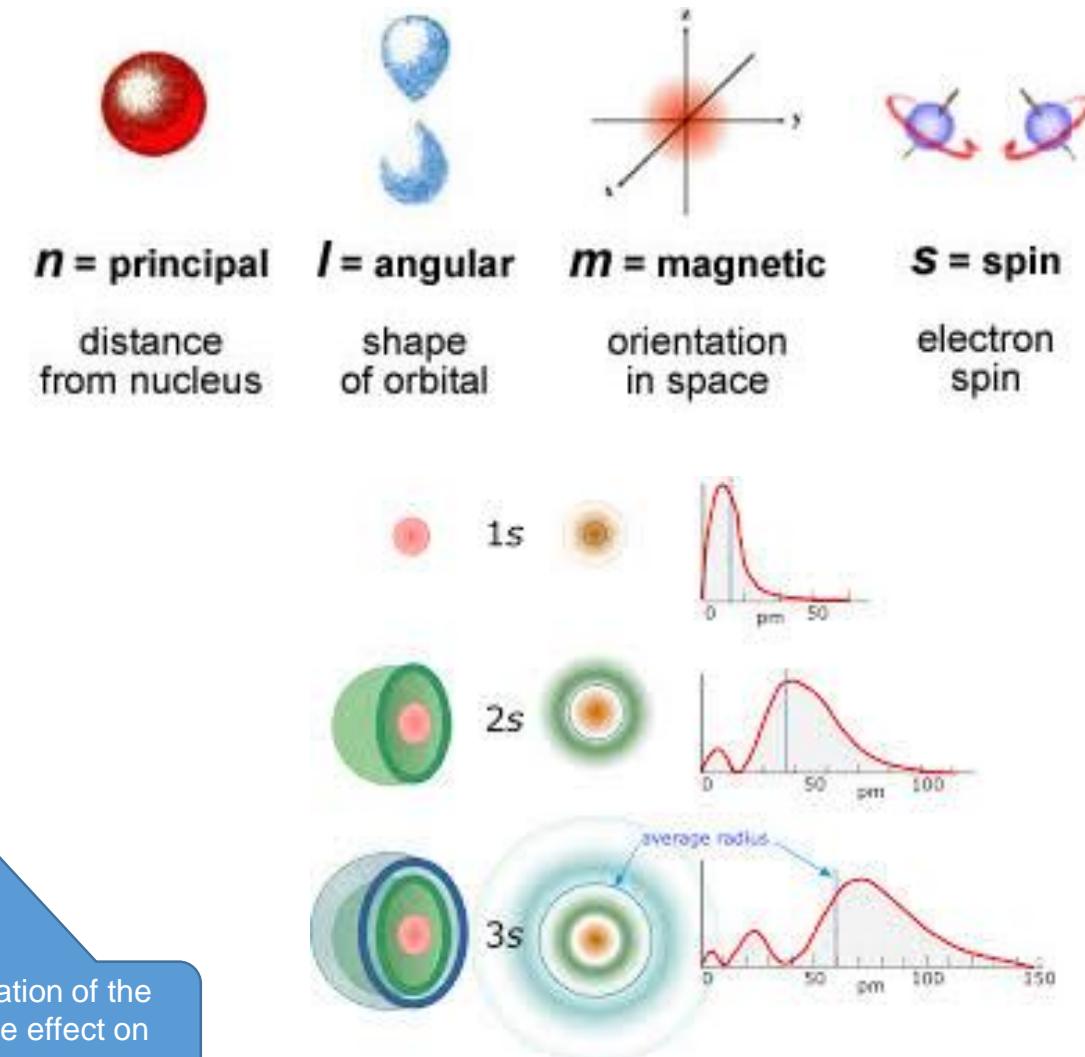


Quantum Numbers

In wave mechanics, every electron in an atom is characterized by four parameters called **quantum numbers**.

The size, shape, and spatial orientation of an electron's probability density (or orbital) are specified by 4 quantum numbers, n, l, m_l, m_s

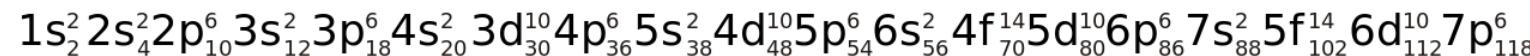
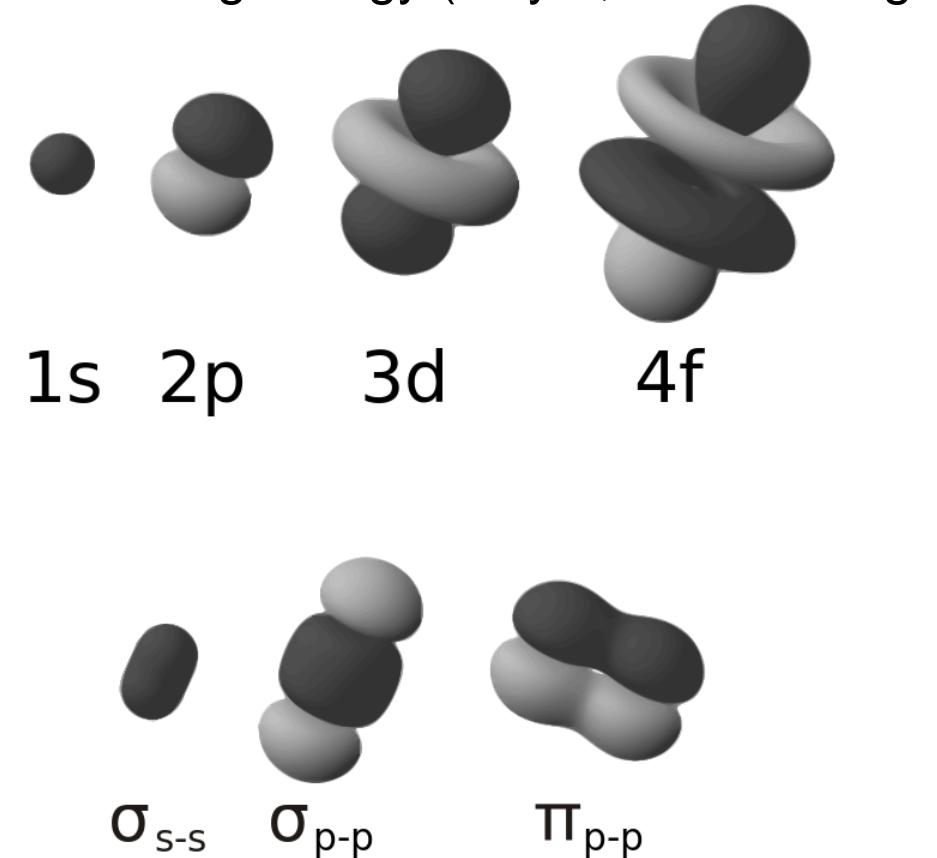
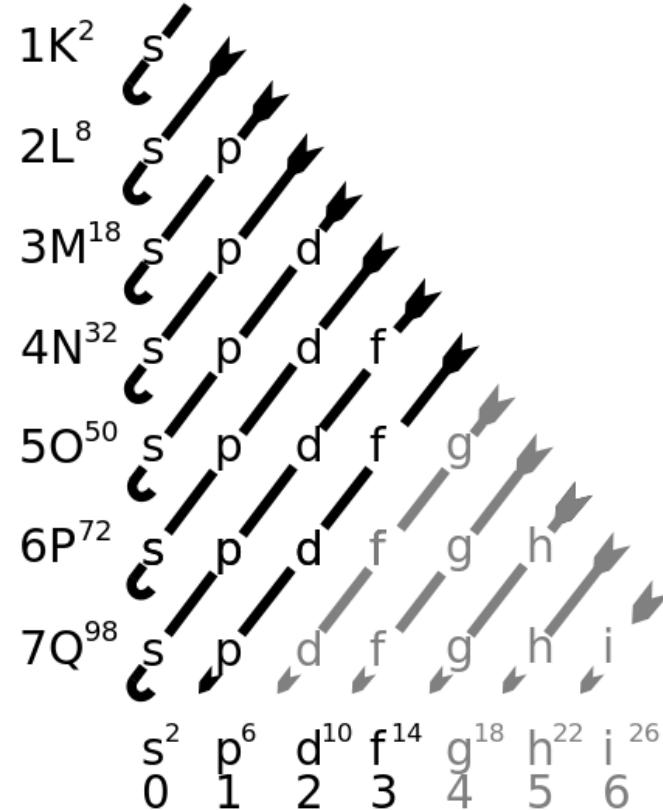
- Principal quantum number (n) = 1, 2, 3, ;
- Azimuthal or subsidiary quantum number (l) = 0, 1, 2, n-1
- Magnetic quantum number (m_l)= 0, 1, 2, ±l ;
- Electron Spin Quantum Number (m_s) = ± ½ called “spin up” or “spin down”





Quantum Numbers: Filling of Orbitals

Electrons that occupy the outermost filled shell – **the valence electrons** – they are responsible for bonding. Electrons fill quantum levels in order of increasing energy (only n, l make a significant difference).



Examples:

Argon, Z = 18: $1s^2 2s^2 2p^6 3s^2 3p^6$

Iron, Z = 26: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$



Electrons in Atom: Filling of Orbitals

<u>Element</u>	<u>Atomic #</u>	<u>Electron configuration</u>
Hydrogen	1	$1s^1$
Helium	2	$1s^2$ (stable)
Lithium	3	$1s^2 2s^1$
Beryllium	4	$1s^2 2s^2$
Boron	5	$1s^2 2s^2 2p^1$
Carbon	6	$1s^2 2s^2 2p^2$
...		...
Neon	10	$1s^2 2s^2 2p^6$ (stable)
Sodium	11	$1s^2 2s^2 2p^6 3s^1$
Magnesium	12	$1s^2 2s^2 2p^6 3s^2$
Aluminum	13	$1s^2 2s^2 2p^6 3s^2 3p^1$
...		...
Argon	18	$1s^2 2s^2 2p^6 3s^2 3p^6$ (stable)
...
Krypton	36	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$ (stable)

Electron configurations where all states within valence electron shell are filled are stable → unreactive inert or noble gas.



Periodic Table

Arranged by atomic number, electron configuration & recurring chemical properties

Periodic Table of the Elements

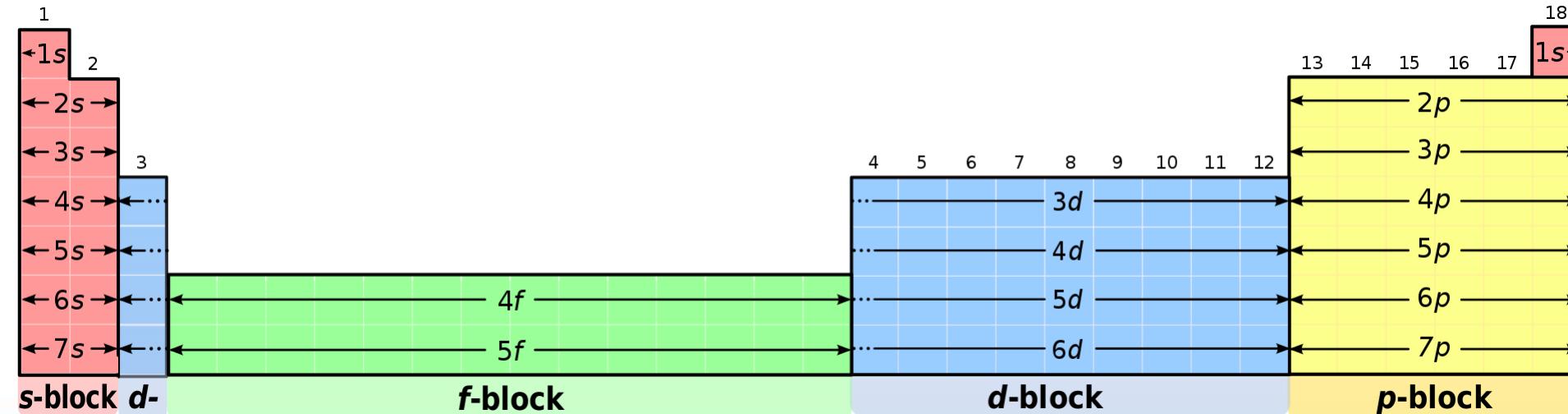
Group	1 1a															18 0		
Period	1 H Hydrogen $1s^1$															He Helium $1s^2$		
1	Li Lithium $1s^2 2s^1$	Be Beryllium $1s^2 2s^2$																
2	Na Sodium $[Ne]3s^1$	Mg Magnesium $[Ne]3s^2$	3 Sc Scandium $[Ar]3d^1 4s^2$	4 Ti Titanium $[Ar]3d^2 4s^2$	5 V Vanadium $[Ar]3d^3 4s^2$	6 Cr Chromium $[Ar]3d^4 4s^2$	7 Mn Manganese $[Ar]3d^5 4s^2$	8 Fe Iron $[Ar]3d^6 4s^2$	9 Co Cobalt $[Ar]3d^7 4s^2$	10 Ni Nickel $[Ar]3d^8 4s^2$	11 Cu Copper $[Ar]3d^9 4s^1$	12 Zn Zinc $[Ar]3d^{10} 4s^2$	13 Al Aluminum $[Ne]3s^2 p^1$	14 Si Silicon $[Ne]3s^2 p^2$	15 P Phosphorus $[Ne]3s^2 p^3$	16 S Sulfur $[Ne]3s^2 p^4$	17 Cl Chlorine $[Ne]3s^2 p^5$	18 Ar Argon $[Ne]3s^2 p^6$
3	19 K Potassium $[Ar]4s^1$	20 Ca Calcium $[Ar]4s^2$	21 Sc Scandium $[Ar]3d^1 4s^2$	22 Ti Titanium $[Ar]3d^2 4s^2$	23 V Vanadium $[Ar]3d^3 4s^2$	24 Cr Chromium $[Ar]3d^4 4s^2$	25 Mn Manganese $[Ar]3d^5 4s^2$	26 Fe Iron $[Ar]3d^6 4s^2$	27 Co Cobalt $[Ar]3d^7 4s^2$	28 Ni Nickel $[Ar]3d^8 4s^2$	29 Cu Copper $[Ar]3d^9 4s^1$	30 Zn Zinc $[Ar]3d^{10} 4s^2$	31 Ga Gallium $[Ar]3d^1 4s^2 p^1$	32 Ge Germanium $[Ar]3d^1 4s^2 p^2$	33 As Arsenic $[Ar]3d^1 4s^2 p^3$	34 Se Selenium $[Ar]3d^1 4s^2 p^4$	35 Br Bromine $[Ar]3d^1 4s^2 p^5$	36 Kr Krypton $[Ar]3d^1 4s^2 p^6$
4	37 Rb Rubidium $[Kr]5s^1$	38 Sr Strontium $[Kr]5s^2$	39 Y Yttrium $[Kr]4d^1 5s^2$	40 Zr Zirconium $[Kr]4d^2 5s^2$	41 Nb Niobium $[Kr]4d^3 5s^2$	42 Mo Molybdenum $[Kr]4d^4 5s^2$	43 Tc Technetium $[Kr]4d^5 5s^2$	44 Ru Ruthenium $[Kr]4d^6 5s^2$	45 Rh Rhodium $[Kr]4d^7 5s^2$	46 Pd Palladium $[Kr]4d^8 5s^2$	47 Ag Silver $[Kr]4d^9 5s^2$	48 Cd Cadmium $[Kr]4d^{10} 5s^2$	49 In Indium $[Kr]4d^{10} 5s^2 p^1$	50 Sn Tin $[Kr]4d^{10} 5s^2 p^2$	51 Sb Antimony $[Kr]4d^{10} 5s^2 p^3$	52 Te Tellurium $[Kr]4d^{10} 5s^2 p^4$	53 I Iodine $[Kr]4d^{10} 5s^2 p^5$	54 Xe Xenon $[Kr]4d^{10} 5s^2 p^6$
5	55 Cs Cesium $[Xe]6s^1$	56 Ba Barium $[Xe]6s^2$	72 Hf Hafnium $[Xe]4f^1 5d^6 6s^2$	73 Ta Tantalum $[Xe]4f^1 5d^6 6s^2$	74 W Tungsten $[Xe]4f^1 5d^6 6s^2$	75 Re Rhenium $[Xe]4f^1 5d^6 6s^2$	76 Os Osmium $[Xe]4f^1 5d^6 6s^2$	77 Ir Iridium $[Xe]4f^1 5d^6 6s^2$	78 Pt Platinum $[Xe]4f^1 5d^6 6s^1$	79 Au Gold $[Xe]4f^1 5d^6 6s^1$	80 Hg Mercury $[Xe]4f^1 5d^6 6s^1$	81 Tl Thallium $[Xe]4f^1 5d^6 6s^1 p^1$	82 Pb Lead $[Xe]4f^1 5d^6 6s^1 p^2$	83 Bi Bismuth $[Xe]4f^1 5d^6 6s^1 p^3$	84 Po Polonium $[Xe]4f^1 5d^6 6s^1 p^4$	85 At Astatine $[Xe]4f^1 5d^6 6s^1 p^5$	86 Rn Radon $[Xe]4f^1 5d^6 6s^1 p^6$	
6	87 Fr Francium $[Rn]5f^7 s^1$	88 Ra Radium $[Rn]5f^7 s^2$	104 Rf Rutherfordium $[Rn]5f^6 6d^1 7s^2$	105 Db Dubnium $[Rn]5f^6 6d^1 7s^2$	106 Sg Seaborgium $[Rn]5f^6 6d^1 7s^2$	107 Bh Bohrium $[Rn]5f^6 6d^1 7s^2$	108 Hs Hassium $[Rn]5f^6 6d^1 7s^2$	109 Mt Meitnerium $[Rn]5f^6 6d^1 7s^2$	110 Ds Darmstadtium $[Rn]5f^6 6d^1 7s^2$	111 Rg Roentgenium $[Rn]5f^6 6d^1 7s^2$	112 Cn Copernicium $[Rn]5f^6 6d^1 7s^2$	113 Uut Ununtrium $[Rn]5f^6 6d^1 7s^2$	114 Fl Flerovium $[Rn]5f^6 6d^1 7s^2$	115 Uup Ununpentium $[Rn]5f^6 6d^1 7s^2$	116 Lv Livermorium $[Rn]5f^6 6d^1 7s^2$	117 Uus Ununseptium $[Rn]5f^6 6d^1 7s^2$	118 Uuo Ununoctium $[Rn]5f^6 6d^1 7s^2$	
7	Aa -Solid	57 La Lanthanum $[Xe]5d^1 6s^2$	58 Ce Cerium $[Xe]4f^1 5d^1 6s^2$	59 Pr Praseodymium $[Xe]4f^1 5d^2 6s^2$	60 Nd Neodymium $[Xe]4f^1 5d^3 6s^2$	61 (145) Pm Promethium $[Xe]4f^1 5d^4 6s^2$	62 150.36 Sm Samarium $[Xe]4f^1 5d^5 6s^2$	63 151.96 Eu Europium $[Xe]4f^1 5d^6 6s^2$	64 157.25 Gd Gadolinium $[Xe]4f^1 5d^7 6s^2$	65 158.93 Tb Terbium $[Xe]4f^1 5d^8 6s^2$	66 162.50 Dy Dysprosium $[Xe]4f^1 5d^9 6s^2$	67 164.93 Ho Holmium $[Xe]4f^1 5d^10 6s^2$	68 167.26 Er Erbium $[Xe]4f^1 5d^11 6s^2$	69 168.93 Tm Thulium $[Xe]4f^1 5d^12 6s^2$	70 173.04 Yb Ytterbium $[Xe]4f^1 5d^13 6s^2$	71 174.97 Lu Lutetium $[Xe]4f^1 5d^14 6s^2$		
Aa -Gas	◆	89 (227) Ac Actinium $[Rn]5f^6 7s^2$	90 232.04 Th Thorium $[Rn]5f^6 7s^2$	91 231.04 Pa Protactinium $[Rn]5f^6 6d^1 7s^2$	92 238.03 U Uranium $[Rn]5f^6 6d^2 7s^2$	93 (237) Np Neptunium $[Rn]5f^6 6d^3 7s^2$	94 (244) Pu Plutonium $[Rn]5f^6 6d^4 7s^2$	95 (243) Am Americium $[Rn]5f^6 6d^5 7s^2$	96 (247) Cm Curium $[Rn]5f^6 6d^6 7s^2$	97 (247) Bk Berkelium $[Rn]5f^6 6d^7 7s^2$	98 (251) Cf Californium $[Rn]5f^6 6d^8 7s^2$	99 (252) Es Einsteinium $[Rn]5f^6 6d^9 7s^2$	100 (257) Fm Fermium $[Rn]5f^6 6d^10 7s^2$	101 (258) Md Mendelevium $[Rn]5f^6 6d^11 7s^2$	102 (259) No Nobelium $[Rn]5f^6 6d^12 7s^2$	103 (262) Lr Lawrencium $[Rn]5f^6 6d^13 7s^2$		

Aa -Solid
Aa -Gas
Aa -Liquid
Aa - Synthetically Prepared



Electrons in Atom: Filling of Orbitals

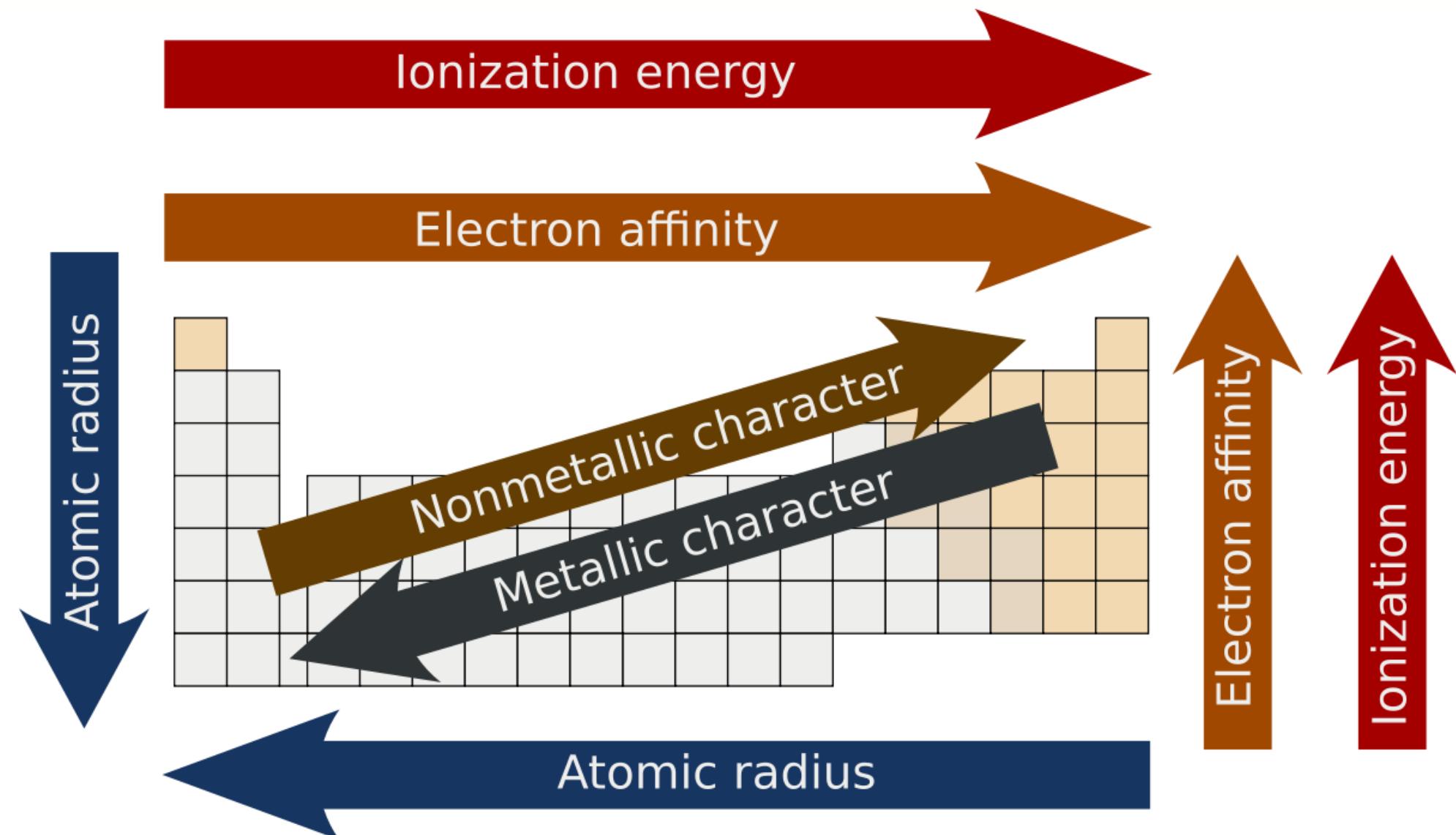
Group Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
1	1 H																2 He		
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne	
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	
5	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	
6	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
7	87 Fr	88 Ra	89 Ac	*	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og





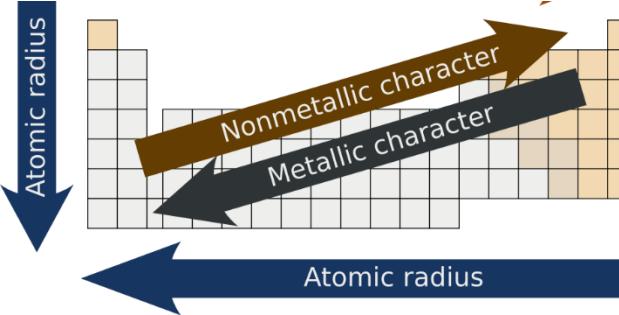
Electrons in Atom: Physical and Chemical properties

- **Ionization energy** is the minimum amount of energy required to remove the valence electron, of an isolated neutral gaseous atom or molecule
- **Electron affinity** is defined as the amount of energy released when an electron is attached to a neutral atom or molecule





Periodic Table –Atomic Radius



- Atomic radius increases with increasing period
- Atomic radius decreases with increasing group



These data are taken from Shannon & Prewitt's (S&P) seminal work on "physical" ionic radii, as determined from measurements of real structures. Note that in most cases S&P quote different radii for the same element: the radii vary according to charge and coordination number. We have chosen the most-common charges (oxidation states) and coordination numbers. Where no radius value can be found for a particular element, its radius has been set to a default value of 1 Å and a circle is plotted instead of a rendered sphere.

References: Shannon RD and Prewitt CT (1969) Acta Crystallographica B25:925-946





Electronegativity, χ

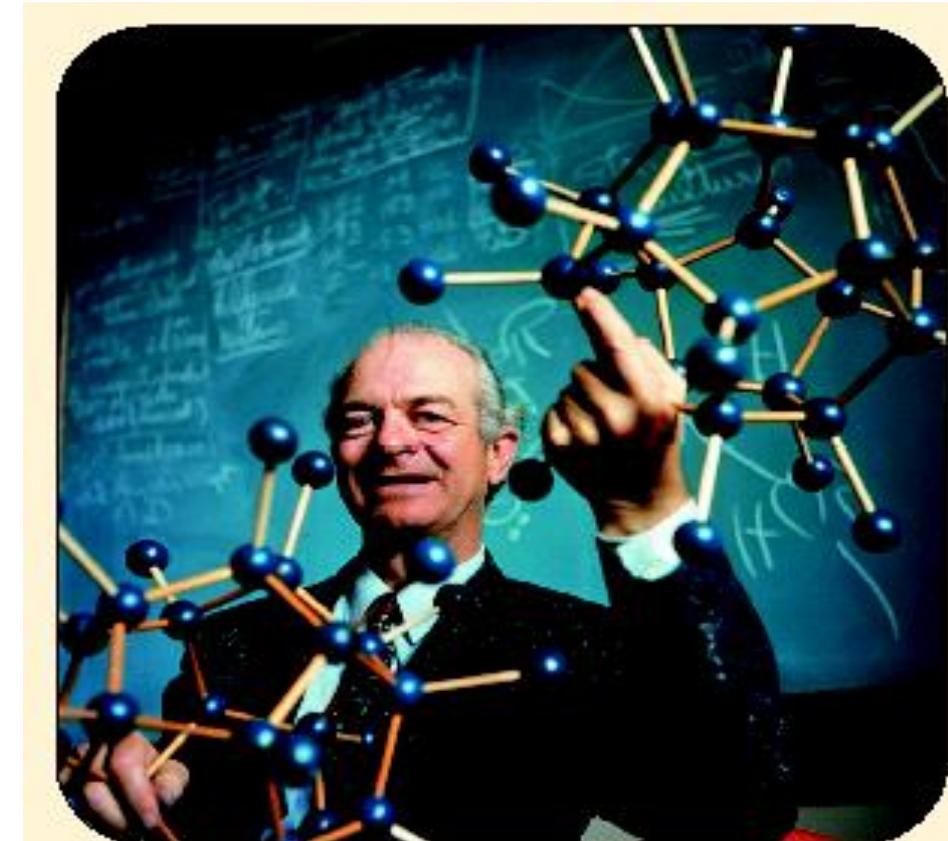
χ is a measure of the ability of an atom in a molecule to attract electrons to itself.

Concept proposed by
Linus Pauling
1901-1994

The only person to receive two unshared Nobel prizes

(for Peace and Chemistry).

Chemistry areas: bonding,
electronegativity, protein structure



▲ Linus Pauling 1901-1994 (Thomas Hollyman/
Photo Researchers, Inc.)



Periodic Table

Periodic Table of the Elements

give up 1e-	give up 2e-	give up 3e-					Accept 2e-	Accept 1e-	Inert gases
1 H Hydrogen 1.01	2 Be Beryllium 9.01								18 He Helium 4.00
3 Li Lithium 6.94	4 Mg Magnesium 24.31								10 Ne Neon 20.18
11 Na Sodium 22.99	12 Al Aluminum 26.98								13 Cl Chlorine 35.45
19 K Potassium 39.10	20 Ca Calcium 40.08	21 Sc Scandium 44.96	22 Ti Titanium 47.88	23 V Vanadium 50.94	24 Cr Chromium 51.99	25 Mn Manganese 54.94	26 Fe Iron 55.93	27 Co Cobalt 58.93	28 Ni Nickel 58.69
37 Rb Rubidium 84.49	38 Sr Strontium 87.62	39 Y Yttrium 88.91	40 Zr Zirconium 91.22	41 Nb Niobium 92.91	42 Mo Molybdenum 95.94	43 Tc Technetium 98.91	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.91	46 Pd Palladium 106.42
55 Cs Cesium 132.91	56 Ba Barium 137.33	57-71 Lanthanides	72 Hf Hafnium 178.49	73 Ta Tantalum 180.95	74 W Tungsten 183.85	75 Re Rhenium 186.21	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08
87 Fr Francium 223.02	88 Ra Radium 226.03	89-103 Actinides	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Berkelium [264]	108 Hs Hassium [269]	109 Mt Methylmercury [268]	110 Ds Darmstadtium [269]
									111 Rg Roentgenium [272]
									112 Cn Copernicium [277]
									113 Uut Ununtrium unknown
									114 Fl Flerovium [289]
									115 Uup Ununpentium unknown
									116 Lv Livermorium [298]
									117 Uus Ununseptium unknown
									118 Uuo Ununoctium unknown

Electropositive elements:

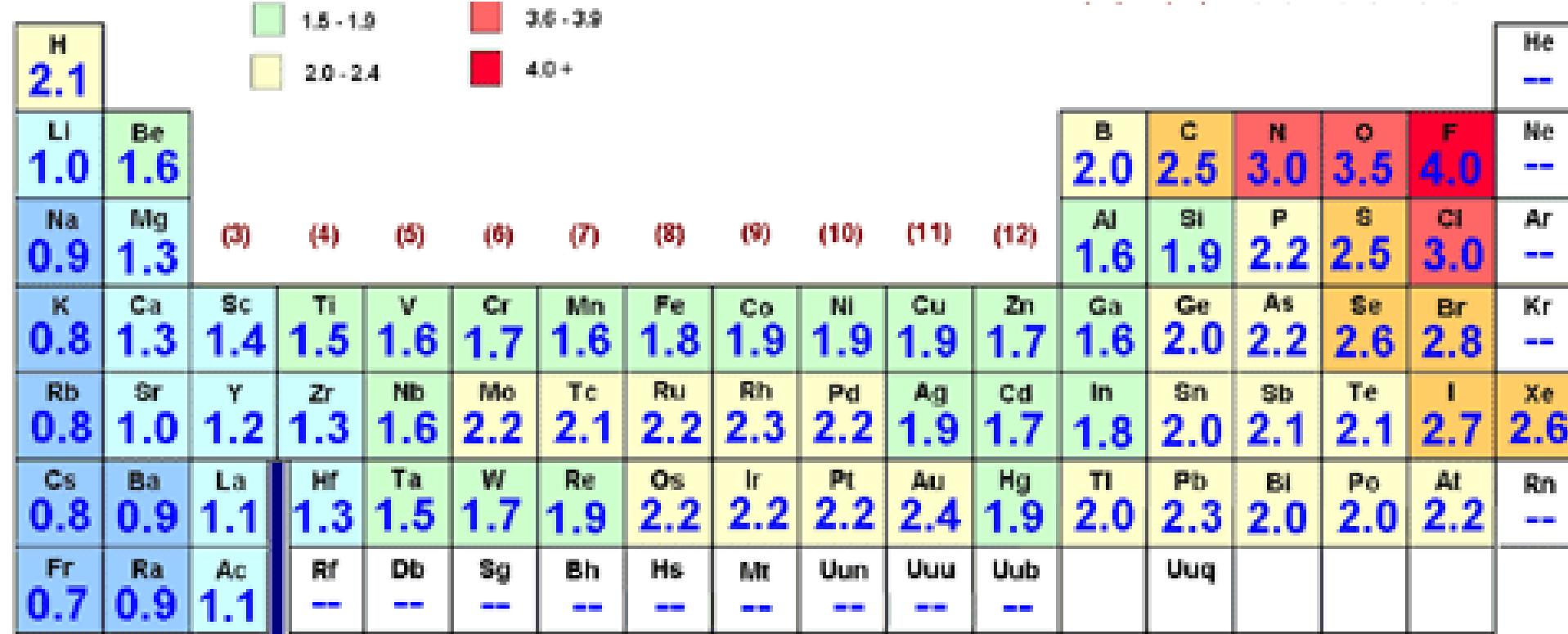
Readily give up electrons to become + ions.

Electronegative elements:

Readily acquire electrons to become - ions.



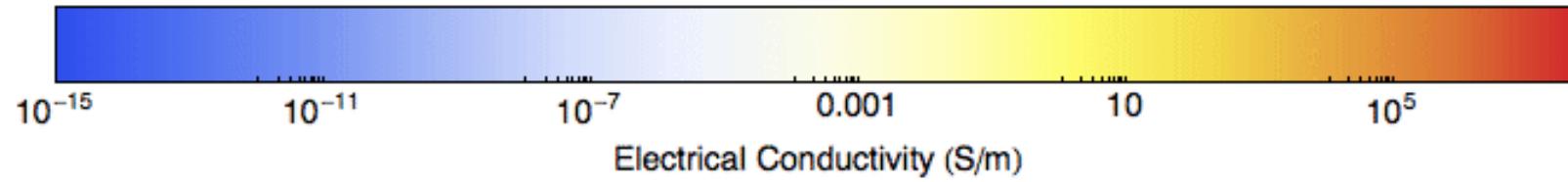
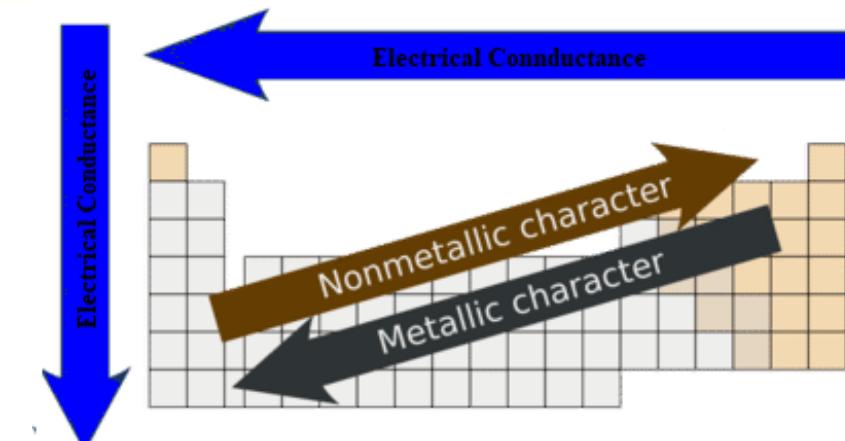
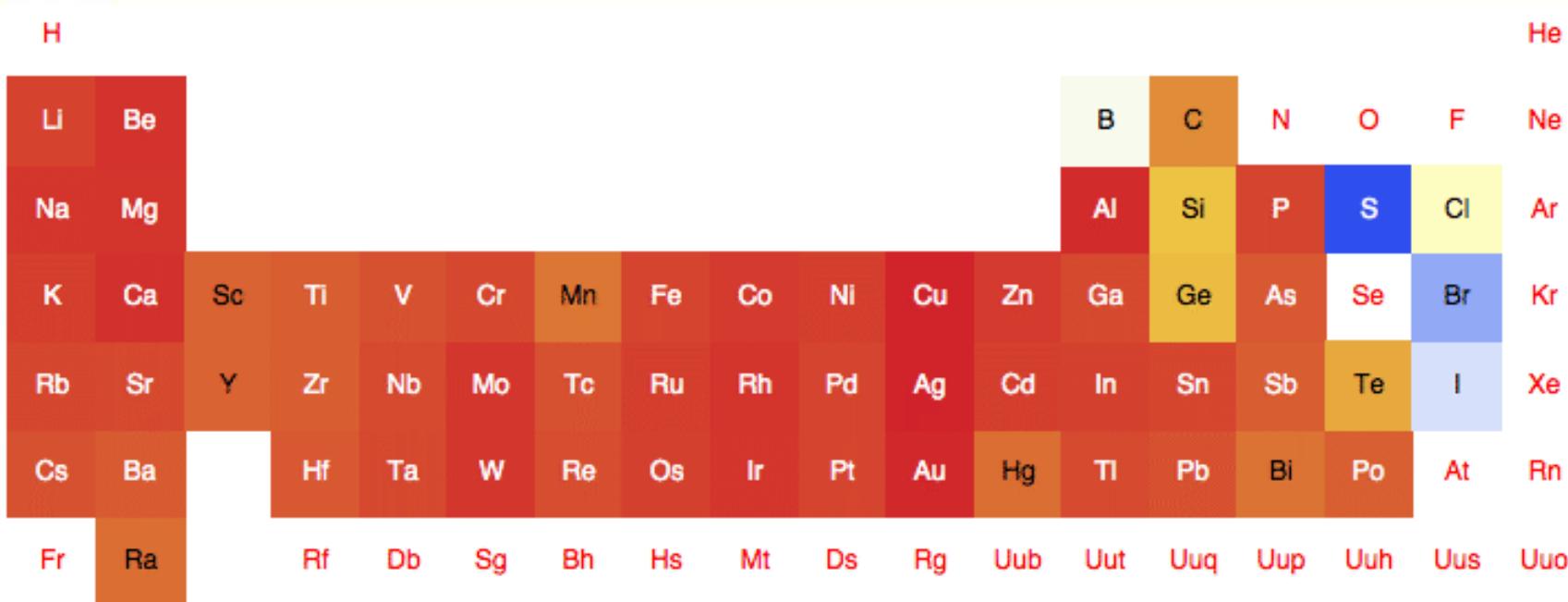
Periodic Table - Electronegativity



- Electronegativity** - a measure of how willing atoms are to accept electrons
- Subshells with one electron** → low electronegativity
- Subshells with one missing electron** → high electronegativity
- Electronegativity increases from left to right**
- Metals are electropositive** – they can give up their few valence electrons to become positively charged ions



Periodic Table – Electrical Conductivity





Endangered Elements and their Conservation

1 H
1.008

3 Li
6.941

11 Na
22.99

19 K
39.10

37 Rb
85.47

55 Cs
132.9

87 Fr
(223)

88 Ra
(226)

89 Ac
(227)

104 Rf
(261)

105 Db
(262)

106 Sg
(266)

107 Bh
(264)

108 Hs
(277)

109 Mt
(268)

110 Ds
(281)

111 Rg
(272)

112 Uub
(285)

113 Uut
(284)

114 Uuo
(289)

115 Uup
(288)

116 Uuh
(292)

117 Uus
(291)

118 Uuo
(294)

58 Ce
140.1

59 Pr
140.9

60 Nd
144.2

61 Pm
(147)

62 Sm
150.4

63 Eu
152

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

71 Lu
175

96 Cm
(247)

97 Bk
(247)

98 Cf
(249)

99 Es
(254)

100 Fm
(253)

101 Md
(256)

102 No
(254)

103 Lr
(262)

Many energy storage technologies currently rely on Lithium; alternative technologies are needed



2 He
4.003

5 B
10.81

6 C
12.01

7 N
14.01

8 O
16.00

9 F
19.00

10 Ne
39.95

13 Al
26.98

14 Si
28.09

15 P
30.97

16 S
32.07

17 Cl
35.45

18 Ar
39.95

Phosphorus is an essential plant nutrient and a major constituent of fertilisers; new methods to obtain phosphorus are needed



Indium is used in some solar cells and display technologies; alternative materials are needed



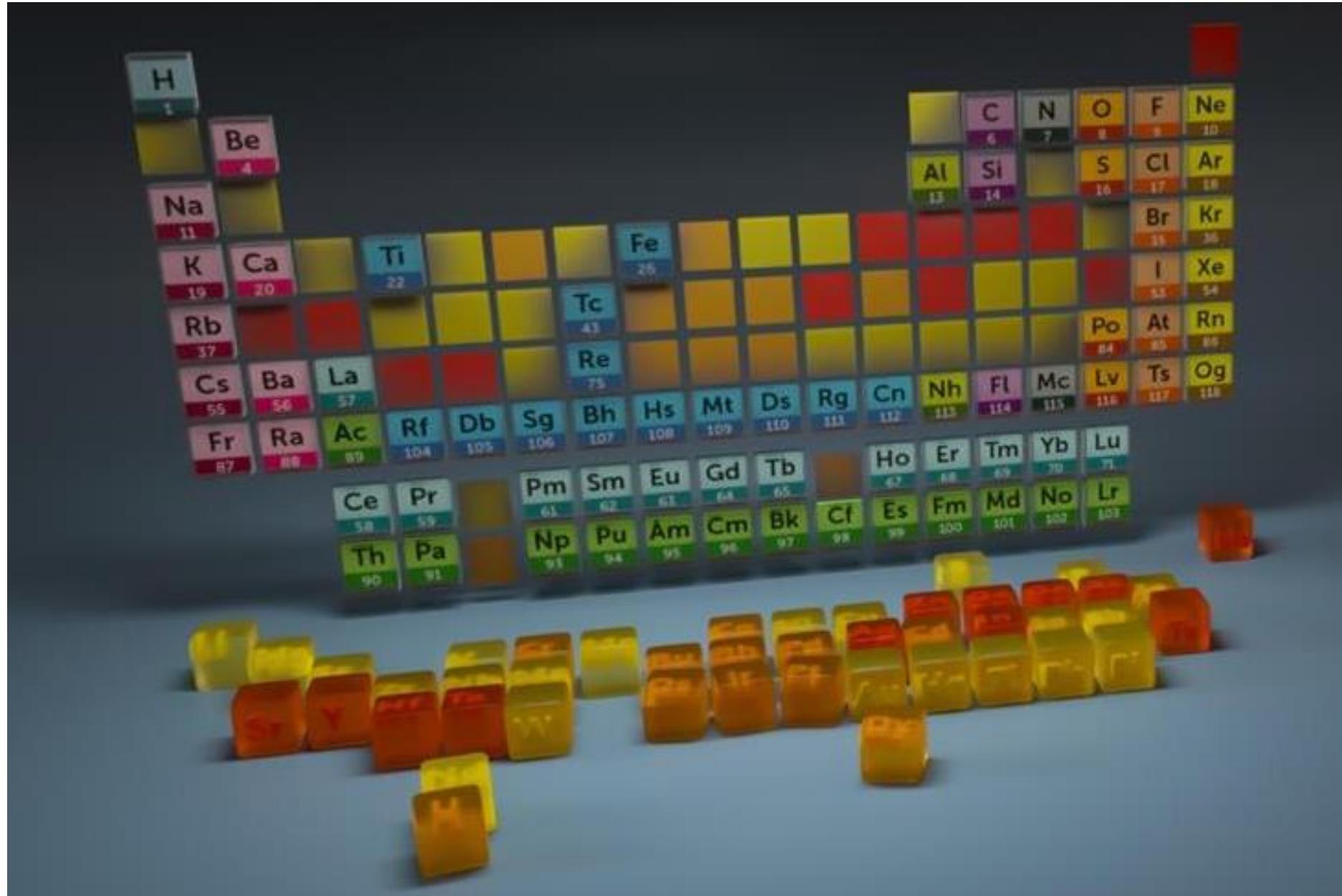
■ Serious threat in the next 100 years

■ Rising threat from increased use

■ Limited availability, future risk to supply

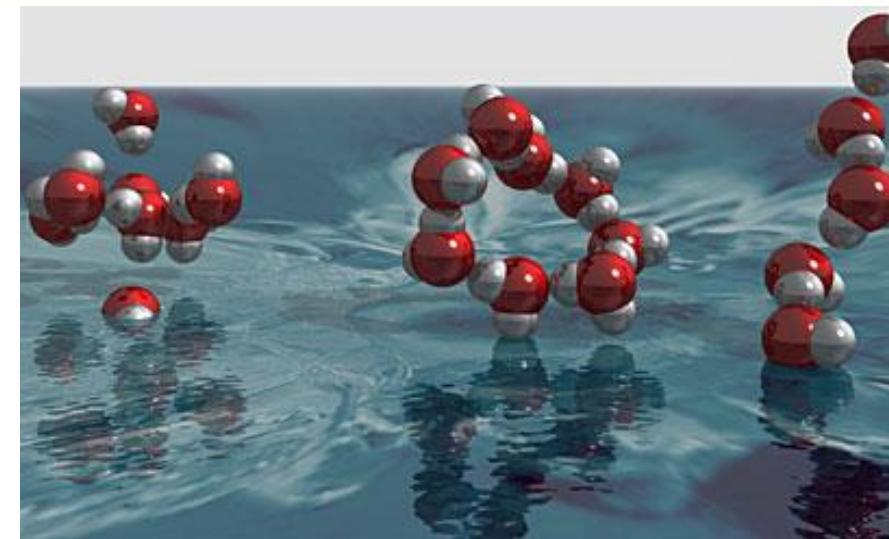


How will we save our endangered elements?

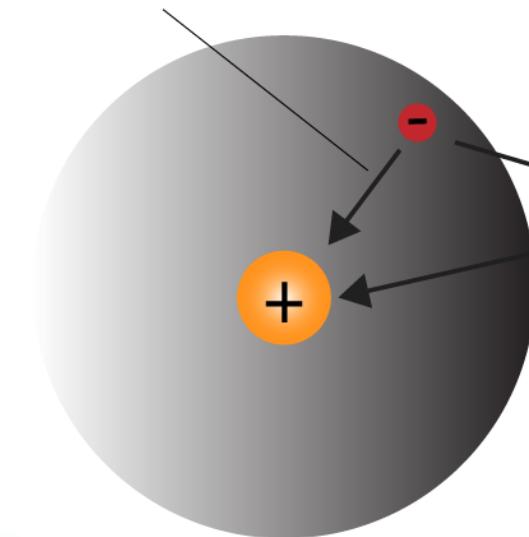




Bonding Forces and Energies



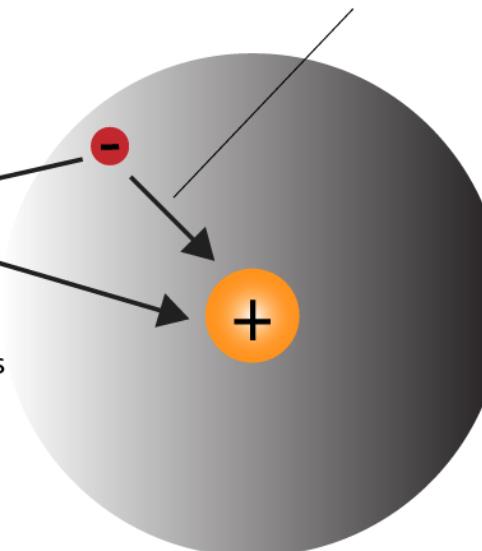
Electron strongly
attracted by the
nucleus



Electron of one atom is
weakly attracted by the
nucleus of the other

This attractive force pulls
the atoms toward
each other

Electron strongly
attracted by the
nucleus



Considering the interaction
between two isolated atoms
as they are brought into
close proximity from an
infinite separation.



Will the atoms collapse on themselves?

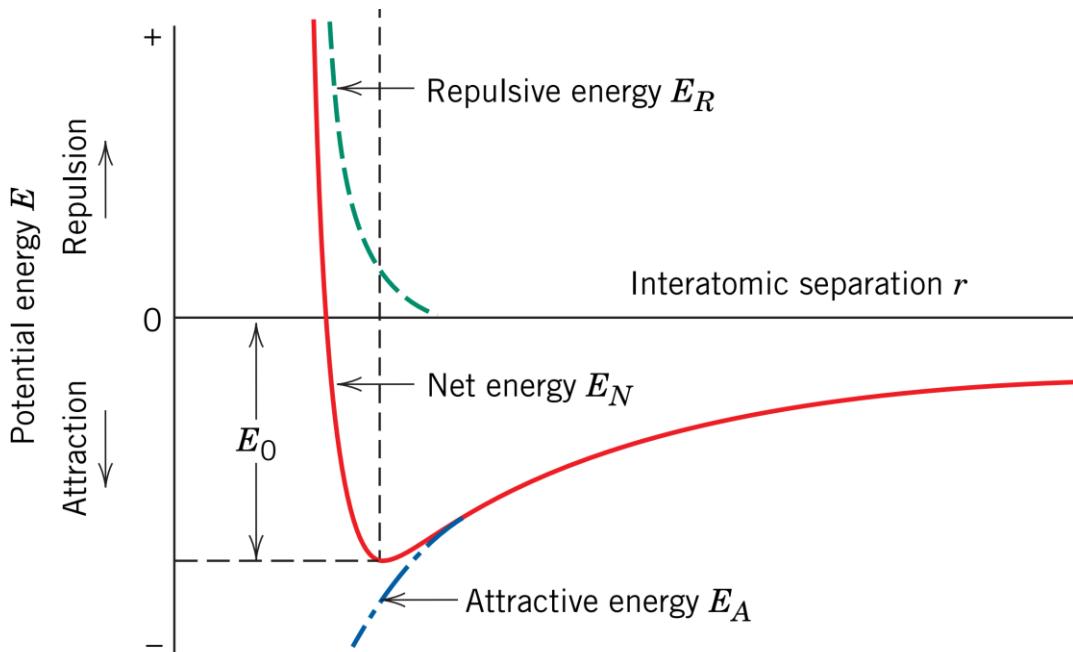
The net force F_N between the two atoms is just the sum of both attractive and repulsive components;

$$F_{Net} = F_{Attractive} + F_{Repulsive}$$

At the state of Equilibrium: F_A and F_R are equal in magnitude but opposite in sign, there is no net force— $F_A + F_R = 0$

It is more convenient to work with the potential energies between two atoms instead of forces. Mathematically, energy (E) and force (F) are related as

$$E = \int F dr$$



For atomic systems

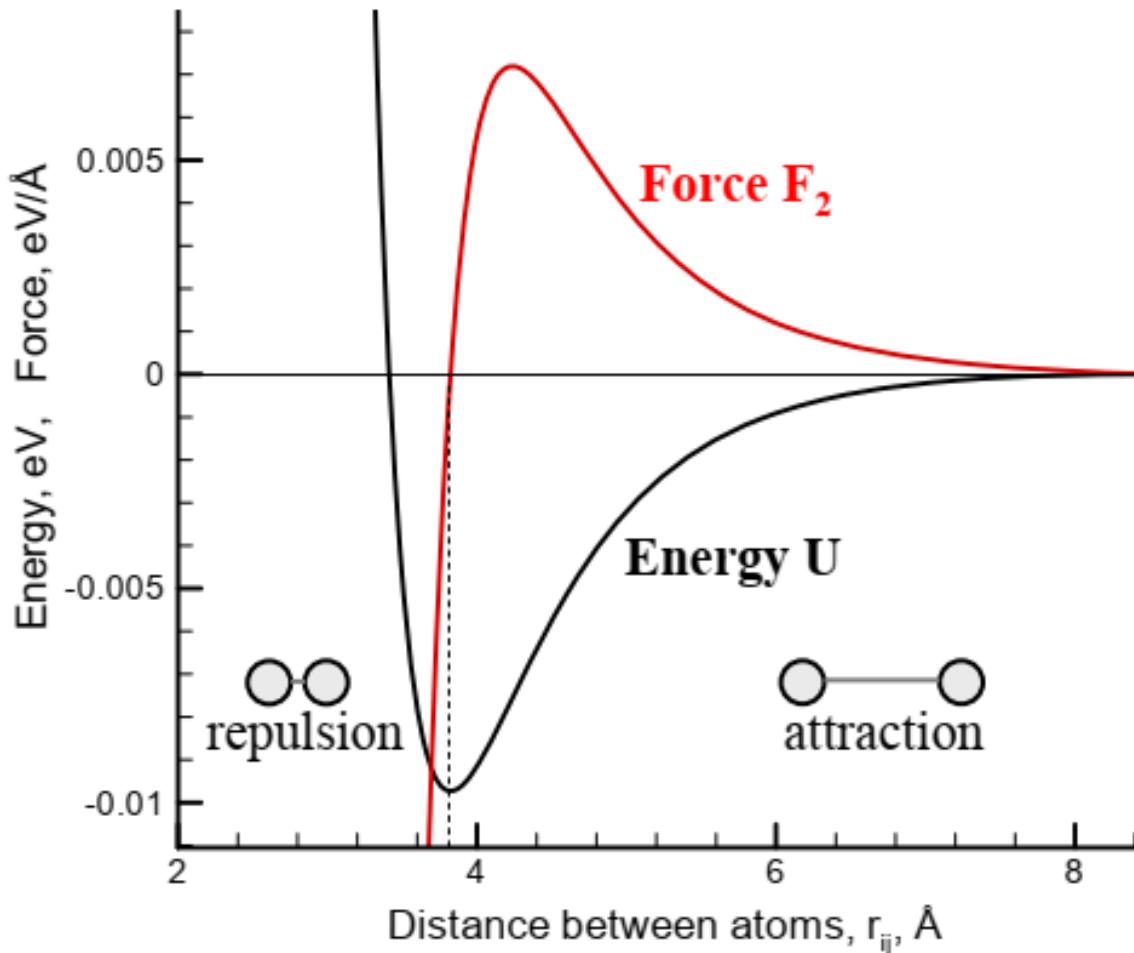
$$E_N = \int_r^\infty F_N dr = \int_r^\infty F_A dr + \int_r^\infty F_R dr = E_A + E_R$$

E_N , E_A , and E_R are, respectively, the net, attractive, and repulsive energies for two isolated and adjacent atoms.

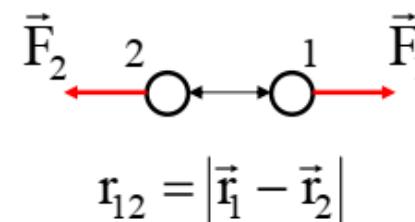
Bonding energy for these two atoms, E_b , corresponds to the energy at this minimum point



Bonding Energies and Forces



$$\vec{F}_1 = -\vec{F}_2 = -\frac{dU(r_{12})}{dr_{12}}$$



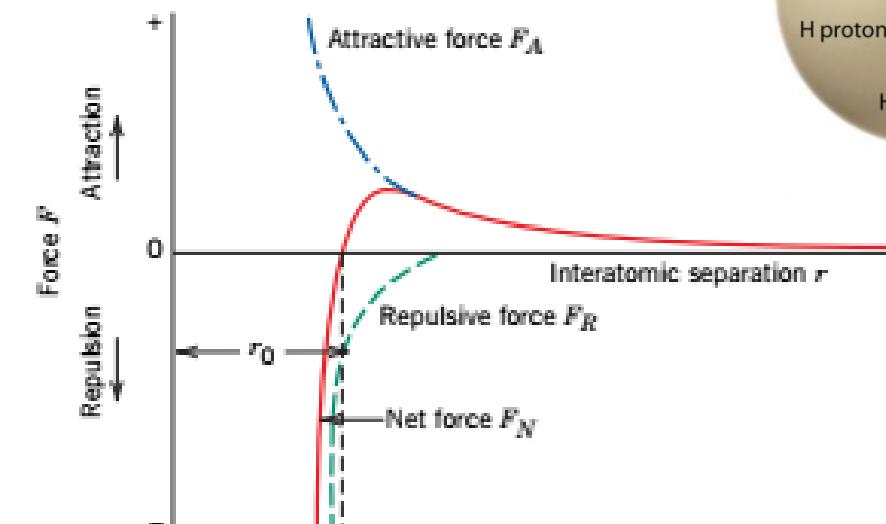
Forces can be calculated from the potential energy of interatomic interaction.
For example, for a system of two atoms (e.g. a diatomic molecule), the potential energy depends only on the distance between the two atoms $U(r_{12})$



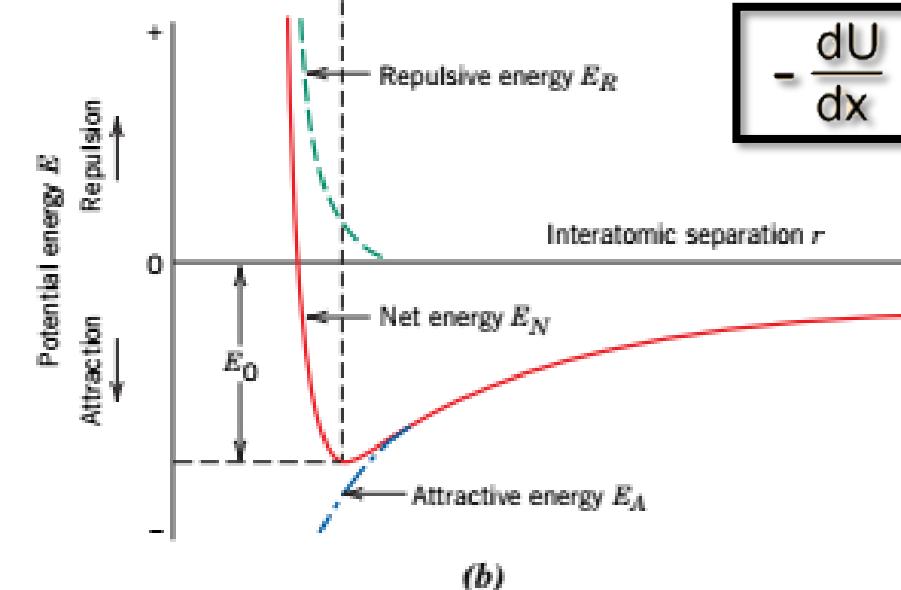
Bonding Forces and Energies

- Considering the interaction between two isolated atoms as they are brought into close proximity from an infinite separation.
- At larger distances, the interactions are negligible.
- As the atoms approach, each exerts forces on the other.
 - **Attractive**
 - **Repulsive**

Ultimately, the outer electron shells of the two atoms begin to overlap, and a strong repulsive force comes into play

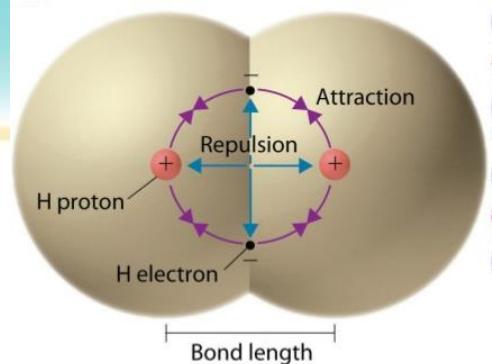


(a)



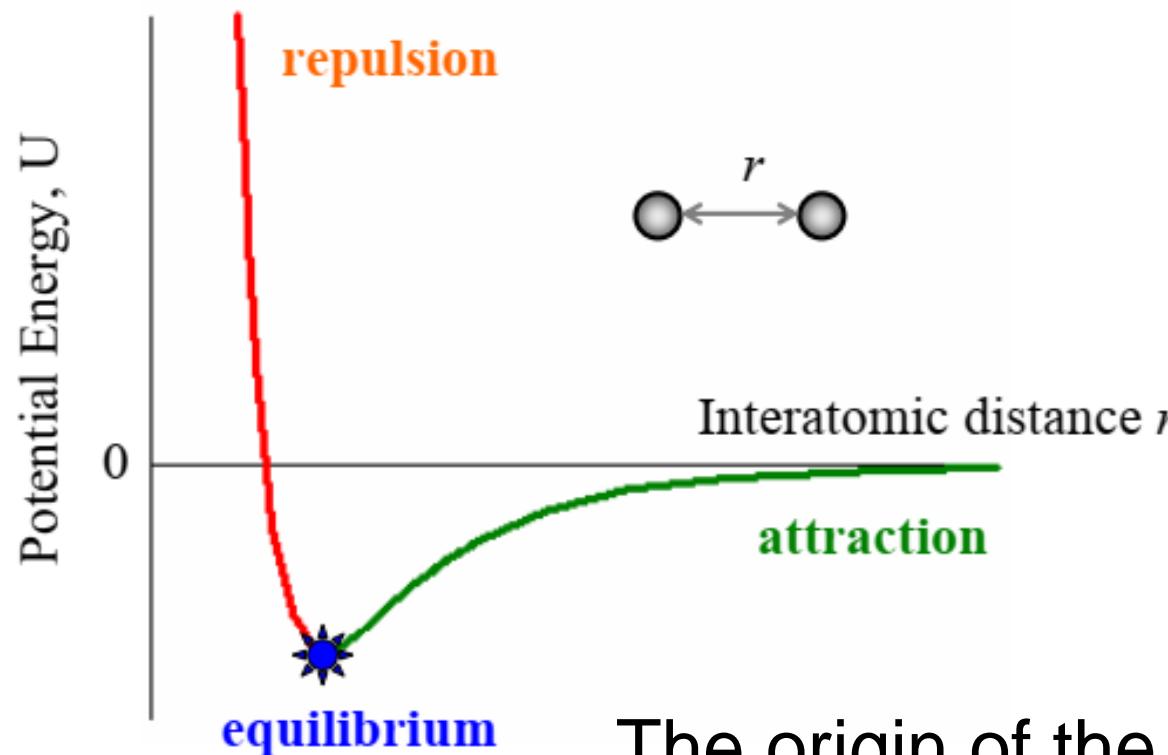
$$-\frac{dU}{dx} = F(x)$$

(b)





Bonding Models



The repulsion between atoms, when they are brought close to each other, is related to the **Pauli principle**: when the electronic clouds surrounding the atoms starts to overlap, the energy of the system increases abruptly.

The origin of the attractive part, dominating at large distances, depends on the particular type of bonding.

https://phet.colorado.edu/sims/html/atomic-interactions/latest/atomic-interactions_en.html

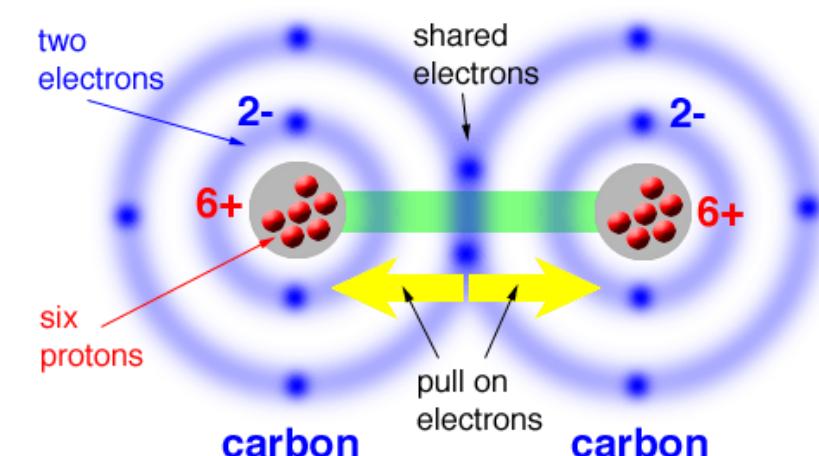
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```



Types of Bonding

- The electronic structure of atoms defines the character of their interaction among each other.
- Filled outer shells result in a stable configuration as in noble inert gases.
- Atoms with incomplete outer shells strive to reach this noble gas configuration by sharing or transferring electrons among each other for maximal stability.
- Strong “primary” bonding results from the electron sharing or transfer.

Hydrogen	H^{\bullet}
Carbon	$\cdot\ddot{\text{C}}\cdot$
Water	$\text{H}\ddot{\text{O}}\text{:}\text{H}$
Ethylene	$\begin{array}{c} \text{H} & \text{H} \\ & \text{C}=\text{C} \\ \text{H} & \text{H} \end{array}$
Acetylene	$\text{H}\text{:}\text{C}\equiv\text{C}\text{:}\text{H}$





The electron volt (eV)

– energy unit convenient for description of atomic bonding

Electron volt - the energy lost / gained by an electron when it is taken through a potential difference of one volt.

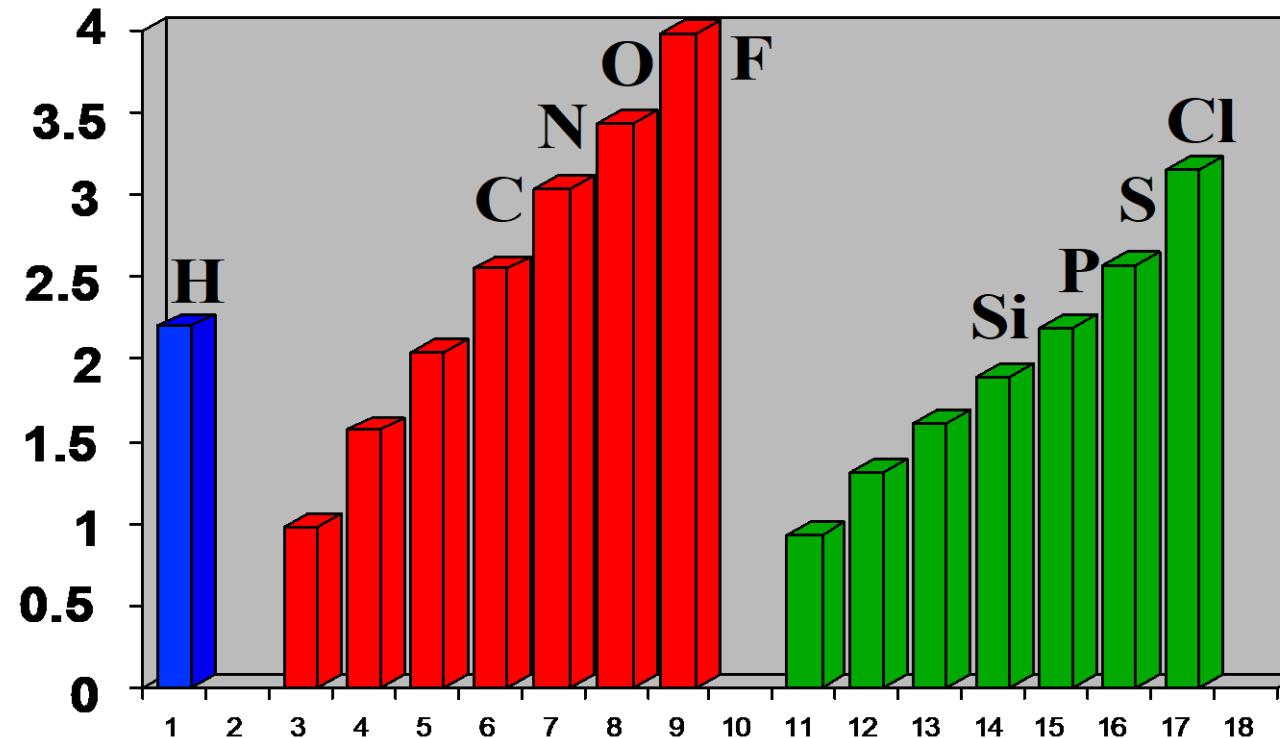
$$E = q \times V$$

for $q = 1.6 \times 10^{-19}$ Coulombs and $V = 1$ volt

$$1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$$



Electronegativity, χ



- F has maximum χ .
- Atom with lowest χ is the center atom in most molecules.
- Relative values of χ determine **BOND POLARITY** (and point of attack on a molecule).

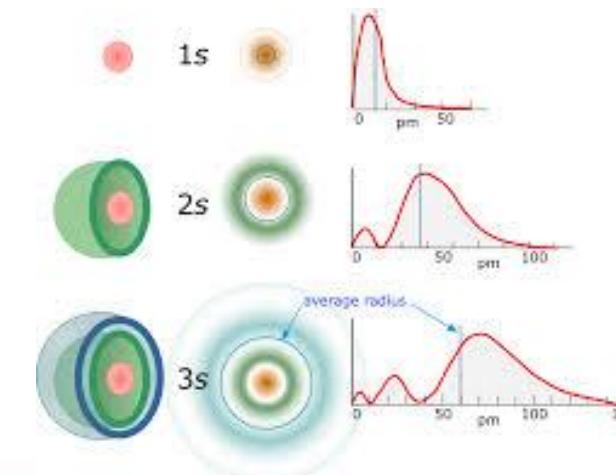
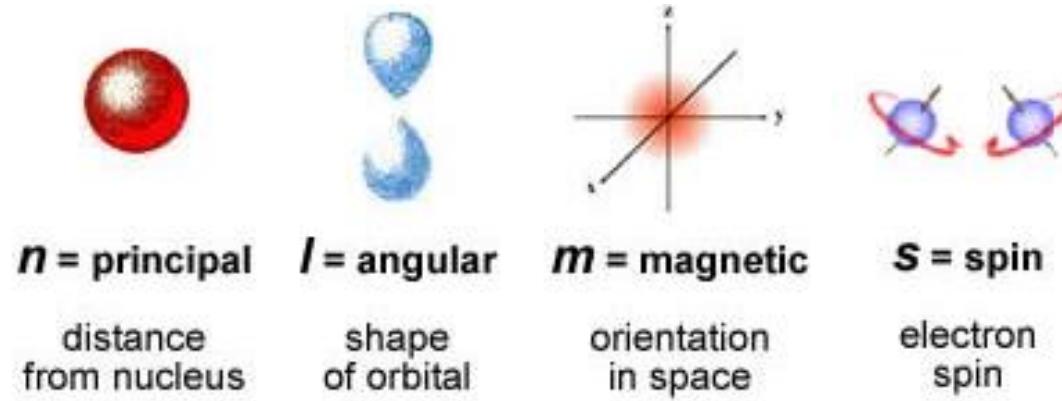


Quantum Numbers

Table 2.1 Summary of the Relationships among the Quantum Numbers n , l , m_l and Numbers of Orbitals and Electrons

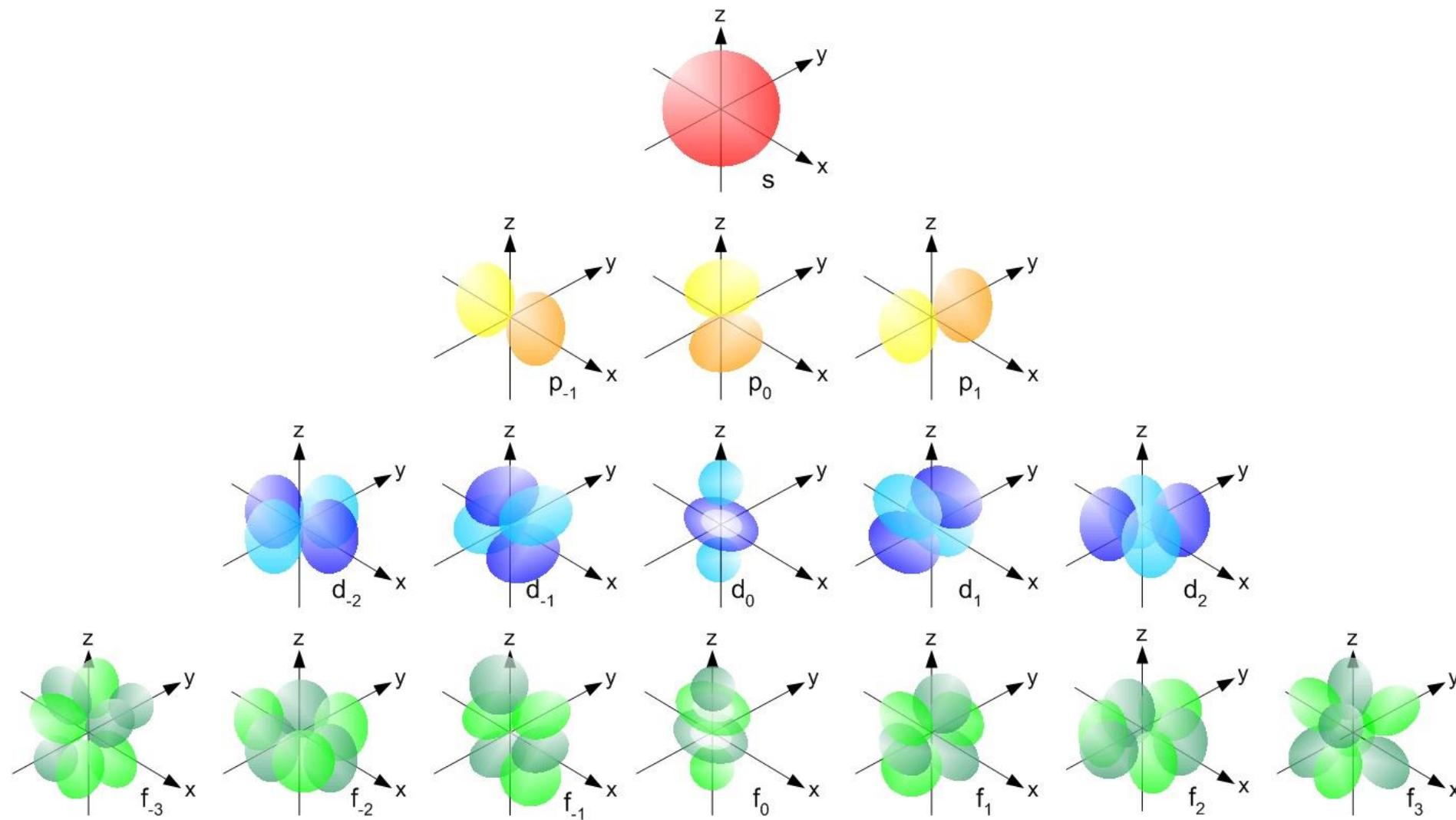
<i>Value of n</i>	<i>Value of l</i>	<i>Values of m_l</i>	<i>Subshell</i>	<i>Number of Orbitals</i>	<i>Number of Electrons</i>
1	0	0	1s	1	2
2	0	0	2s	1	2
	1	-1, 0, +1	2p	3	6
	0	0	3s	1	2
3	1	-1, 0, +1	3p	3	6
	2	-2, -1, 0, +1, +2	3d	5	10
	0	0	4s	1	2
4	1	-1, 0, +1	4p	3	6
	2	-2, -1, 0, +1, +2	4d	5	10
	3	-3, -2, -1, 0, +1, +2, +3	4f	7	14

Source: From J. E. Brady and F. Senese, *Chemistry: Matter and Its Changes*, 4th edition. Reprinted with permission of John Wiley & Sons, Inc.





Quantum Numbers



Orientations and shapes of electron orbitals