ME 254: Materials Engineering

Chapter 2: Atomic Structure and Interatomic Bonding

1st Semester 1435-1436 (Fall 2014)

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Outline

- Atomic structure and electron configurations

- Interatomic bonding: primary and secondary
  - Ionic
  - Covalent
  - Metallic
  - Secondary

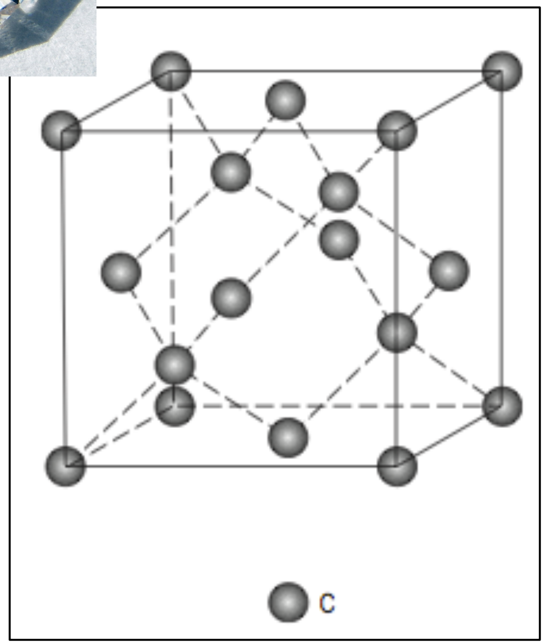
WHY STUDY Atomic Structure and Interatomic Bonding?

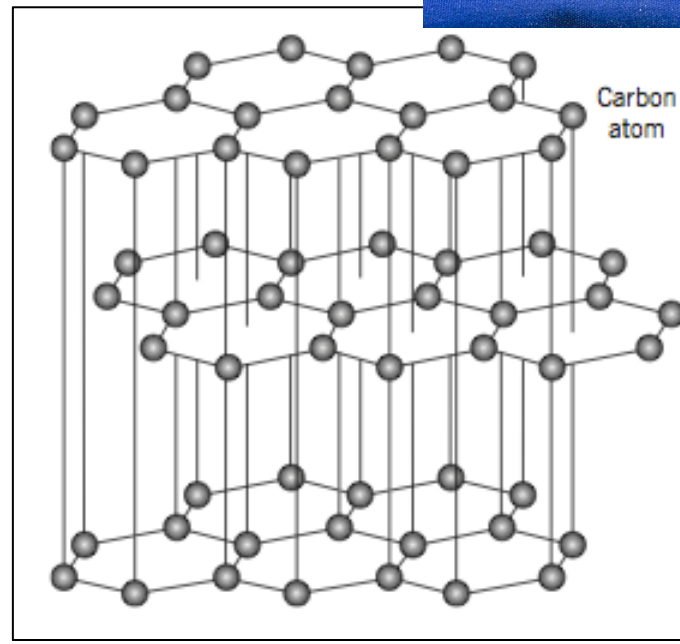
From Chapter 1:

Some of the properties in solid materials strongly depend on the type of atomic structure and interatomic bonding

Carbon

Diamond vs. Graphite





	Diamond	Graphite
Interatomic Bonding:	Strong covalent	Strong covalent + weak van der Waals
Properties:	Extremely hard, very low electrical conductivity	Soft , lubricant, relatively high electrical conductivity

Atomic Structure:

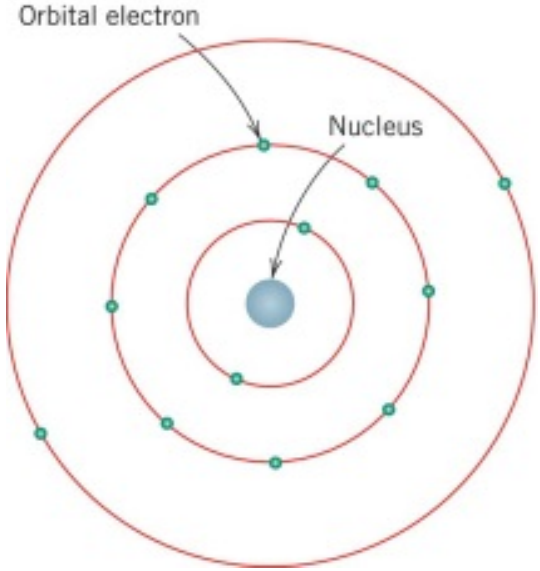


Fig_02_01

Atom

Nucleus

Proton (p^+) & neutron (n^0)

1.6×10^{-9} C
1.673×10^{-27} kg

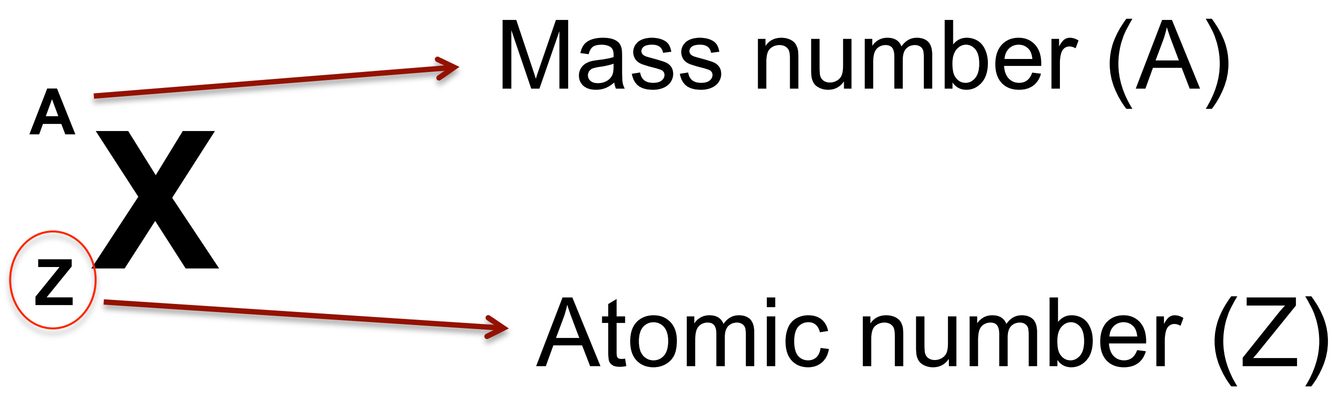
Electron (e^-)

-1.6×10^{-9} C
9.11×10^{-31} kg

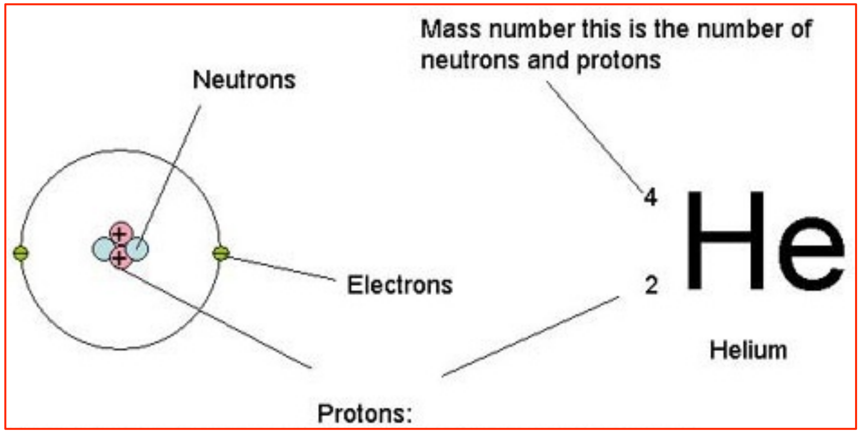
Atomic number (Z) = number of protons (n_p) in nucleus
= number of electrons in neutral species only

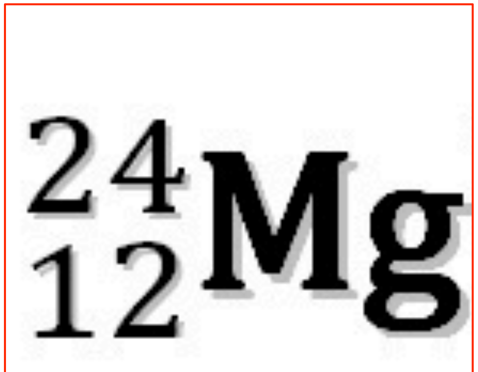
Mass number (A) = number of protons + number of neutron

Chemical Symbol



Example:





Magnesium

Isotopes

For all atoms of a given element, the number of protons is the same but the number of neutrons may be variable.

Isotopes: Atoms of the same element that have different number of neutrons.

Note the following:

1. *Isotopes have the same proton numbers (Because they're from the same element)*
2. *Isotopes have different atomic masses (Because they've different number of neutrons)*

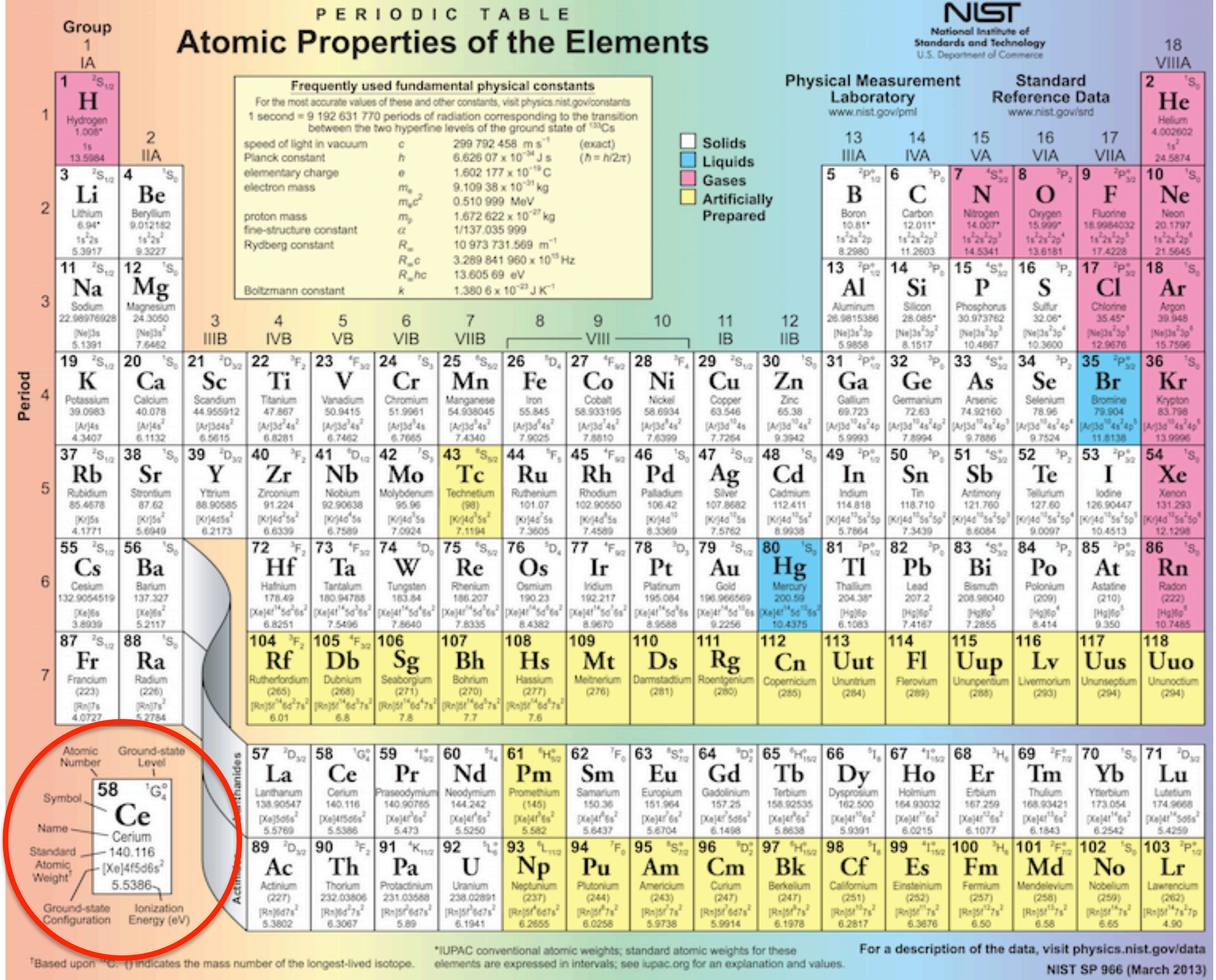
Example:

Carbon-12, (A=12), Carbon-13, (A=13), Carbon-14, (A=14)

Atomic number (Z) for Carbon=6

➔ *No. of neutrons= 6, 7, & 8 for C-12, C-13, & C-14, respectively*

- **Atomic mass:** mass of protons + mass of neutron
- **Atomic mass unit (amu)**: it is a measure of atomic mass defined as 1/12 of the atomic mass of the most common isotopes of carbon, ^{12}C.
- **Atomic weight (relative atomic mass)**: The weighted average of the atomic masses of the atom's naturally occurring isotopes
- In one **mole** of a substance there are 6.023×10^{23} (Avogadro's number) atoms or molecules.
  1 mole ➔ 6.023×10^{23} atoms
- 1 amu/atom= 1 g/mole


PERIODIC TABLE
Atomic Properties of the Elements
NIST National Institute of Standards and Technology U.S. Department of Commerce
Physical Measurement Laboratory www.nist.gov/pml
Standard Reference Data www.nist.gov/srd
Frequently used fundamental physical constants
For the most accurate values of these and other constants, visit physics.nist.gov/constants
1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of 133Cs
speed of light in vacuum c 299 792 458 m s-1 (exact)
Planck constant h 6.626 07 x 10-34 J s (ħ = h/2π)
elementary charge e 1.602 177 x 10-19 C
electron mass me 9.109 38 x 10-31 kg
mec2 0.510 999 MeV
proton mass mp 1.672 622 x 10-27 kg
fine-structure constant α 1/137.035 999
Rydberg constant R∞ 10 973 731.569 m-1
R∞c 3.289 841 960 x 1015 Hz
R∞hc 13.605 69 eV
Boltzmann constant k 1.380 6 x 10-23 J K-1
Solids
Liquids
Gases
Artificially Prepared
Group
Period
1 H Hydrogen 1.008*
2 He Helium 4.002602
3 Li Lithium 6.94*
4 Be Beryllium 9.012182
5 B Boron 10.81*
6 C Carbon 12.011*
7 N Nitrogen 14.007*
8 O Oxygen 15.999*
9 F Fluorine 18.9984032
10 Ne Neon 20.1797
11 Na Sodium 22.98976928
12 Mg Magnesium 24.3050
13 Al Aluminum 26.9815386
14 Si Silicon 28.085*
15 P Phosphorus 30.973762
16 S Sulfur 32.06*
17 Cl Chlorine 35.45*
18 Ar Argon 39.948
19 K Potassium 39.0983
20 Ca Calcium 40.078
21 Sc Scandium 44.955912
22 Ti Titanium 47.867
23 V Vanadium 50.9415
24 Cr Chromium 51.9961
25 Mn Manganese 54.938045
26 Fe Iron 55.845
27 Co Cobalt 58.933195
28 Ni Nickel 58.6934
29 Cu Copper 63.546
30 Zn Zinc 65.38
31 Ga Gallium 69.723
32 Ge Germanium 72.63
33 As Arsenic 74.92160
34 Se Selenium 78.96
35 Br Bromine 79.904
36 Kr Krypton 83.798
37 Rb Rubidium 85.4678
38 Sr Strontium 87.62
39 Y Yttrium 88.90585
40 Zr Zirconium 91.224
41 Nb Niobium 92.90638
42 Mo Molybdenum 95.96
43 Tc Technetium (98)
44 Ru Ruthenium 101.07
45 Rh Rhodium 102.90550
46 Pd Palladium 106.42
47 Ag Silver 107.8682
48 Cd Cadmium 112.411
49 In Indium 114.818
50 Sn Tin 118.710
51 Sb Antimony 121.760
52 Te Tellurium 127.60
53 I Iodine 126.90447
54 Xe Xenon 131.293
55 Cs Cesium 132.9054519
56 Ba Barium 137.327
72 Hf Hafnium 178.49
73 Ta Tantalum 180.94788
74 W Tungsten 183.84
75 Re Rhenium 186.207
76 Os Osmium 190.23
77 Ir Iridium 192.217
78 Pt Platinum 195.084
79 Au Gold 196.966569
80 Hg Mercury 200.59
81 Tl Thallium 204.38*
82 Pb Lead 207.2
83 Bi Bismuth 208.98040
84 Po Polonium (209)
85 At Astatine (210)
86 Rn Radon (222)
87 Fr Francium (223)
88 Ra Radium (226)
104 Rf Rutherfordium (265)
105 Db Dubnium (268)
106 Sg Seaborgium (271)
107 Bh Bohrium (270)
108 Hs Hassium (277)
109 Mt Meitnerium (276)
110 Ds Darmstadtium (281)
111 Rg Roentgenium (280)
112 Cn Copernicium (285)
113 Uut Ununtrium (284)
114 Fl Flerovium (289)
115 Uup Ununpentium (288)
116 Lv Livermorium (293)
117 Uus Ununseptium (294)
118 Uuo Ununoctium (294)
Lanthanides
57 La Lanthanum 138.90547
58 Ce Cerium 140.116
59 Pr Praseodymium 140.90765
60 Nd Neodymium 144.242
61 Pm Promethium (145)
62 Sm Samarium 150.36
63 Eu Europium 151.964
64 Gd Gadolinium 157.25
65 Tb Terbium 158.92535
66 Dy Dysprosium 162.500
67 Ho Holmium 164.93032
68 Er Erbium 167.259
69 Tm Thulium 168.93421
70 Yb Ytterbium 173.054
71 Lu Lutetium 174.9668
Actinides
89 Ac Actinium (227)
90 Th Thorium 232.03806
91 Pa Protactinium 231.03588
92 U Uranium 238.02891
93 Np Neptunium (237)
94 Pu Plutonium (244)
95 Am Americium (243)
96 Cm Curium (247)
97 Bk Berkelium (247)
98 Cf Californium (251)
99 Es Einsteinium (252)
100 Fm Fermium (257)
101 Md Mendelevium (258)
102 No Nobelium (259)
103 Lr Lawrencium (262)
Atomic Number
Ground-state Level
Symbol
Name
Standard Atomic Weight†
Ground-state Configuration
Ionization Energy (eV)
58 Ce Cerium 140.116 [Xe]4f5d6s2 5.5386
†Based upon 12C. ( ) indicates the mass number of the longest-lived isotope.
*IUPAC conventional atomic weights; standard atomic weights for these elements are expressed in intervals; see iupac.org for an explanation and values.
For a description of the data, visit physics.nist.gov/data
NIST SP 966 (March 2013)

Atomic weight:

2.2 Silicon has three naturally-occurring isotopes: 92.23% of ^{28}Si, with an atomic weight of 27.9769 amu, 4.68% of ^{29}Si, with an atomic weight of 28.9765 amu, and 3.09% of ^{30}Si, with an atomic weight of 29.9738 amu. On the basis of these data, confirm that the average atomic weight of Si is 28.0854 amu.

Example 1 (Problem 2.2)

2.2 Silicon has three naturally-occurring isotopes: 92.23% of ^{28}Si, with an atomic weight of 27.9769 amu, 4.68% of ^{29}Si, with an atomic weight of 28.9765 amu, and 3.09% of ^{30}Si, with an atomic weight of 29.9738 amu. On the basis of these data, confirm that the average atomic weight of Si is 28.0854 amu.

Atomic_wieght = 92.23/100 * 27.9769
+ 4.68/100 * 28.9765
+ 3.09/100 * 29.9738
= 28.0854 amu

Example 2:

How many atoms of iron (Fe) in 1 g of Fe?

Atomic weight of Fe is 55.845 g/mol

Avogadro number = 6.023×10^{23}

See Homework 2

Electronic Structure

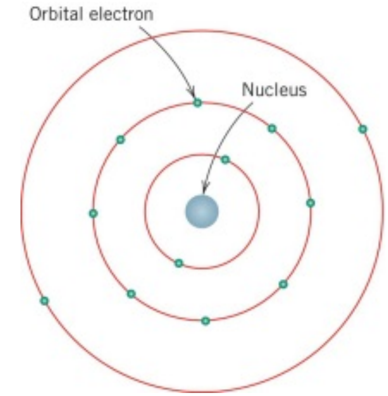


Fig_02_01

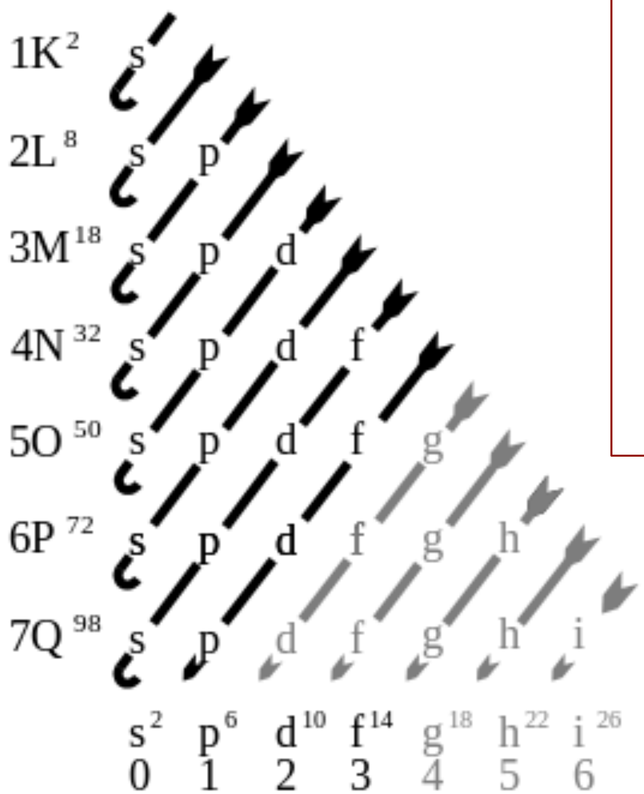
- Electrons are assumed to revolve around the atomic nucleus in discrete orbitals
- Energies of electrons are quantized; that is, electrons are permitted to have only specific values of energy
- Each orbital at discrete energy level is determined by quantum numbers.

Quantum #	Designation
n = principal (energy level-shell)	K, L, M, N, O (1, 2, 3, etc.)
ℓ = subsidiary (orbitals, subshell)	s, p, d, f (0, 1, 2, 3,…, n-1)
m_l = magnetic	1, 3, 5, 7 ($-\ell$ to $+\ell$)
m_s = spin	½, -½

Electronic Structure

Table 2.1 **The Number of Available Electron States in Some of the Electron Shells and Subshells**

Principal Quantum Number n	*Shell Designation*	*Subshells*	*Number of States*	*Number of Electrons*	
				Per Subshell	*Per Shell*
1	*K*	*s*	1	2	2
2	*L*	*s*	1	2	8
		p	3	6	
3	*M*	*s*	1	2	18
		p	3	6	
		d	5	10	
4	*N*	*s*	1	2	32
		p	3	6	
		d	5	10	
		f	7	14	



$1s^{2}_{2}\ 2s^{2}_{4}\ 2p^{6}_{10}\ 3s^{2}_{12}\ 3p^{6}_{18}\ 4s^{2}_{20}\ 3d^{10}_{30}\ 4p^{6}_{36}\ 5s^{2}_{38}\ 4d^{10}_{48}\ 5p^{6}_{54}\ 6s^{2}_{56}\ 4f^{14}_{70}\ 5d^{10}_{80}\ 6p^{6}_{86}\ 7s^{2}_{88}\ 5f^{14}_{102}\ 6d^{10}_{112}\ 7p^{6}_{118}$

See Table 2.2 for a list of the electron configurations for some common elements

- **Valence electrons:** The electrons in the outermost occupied electron shell, which participate in inter- atomic bonding.

- Many of the physical and chemical properties of solids are based on the valence electrons.

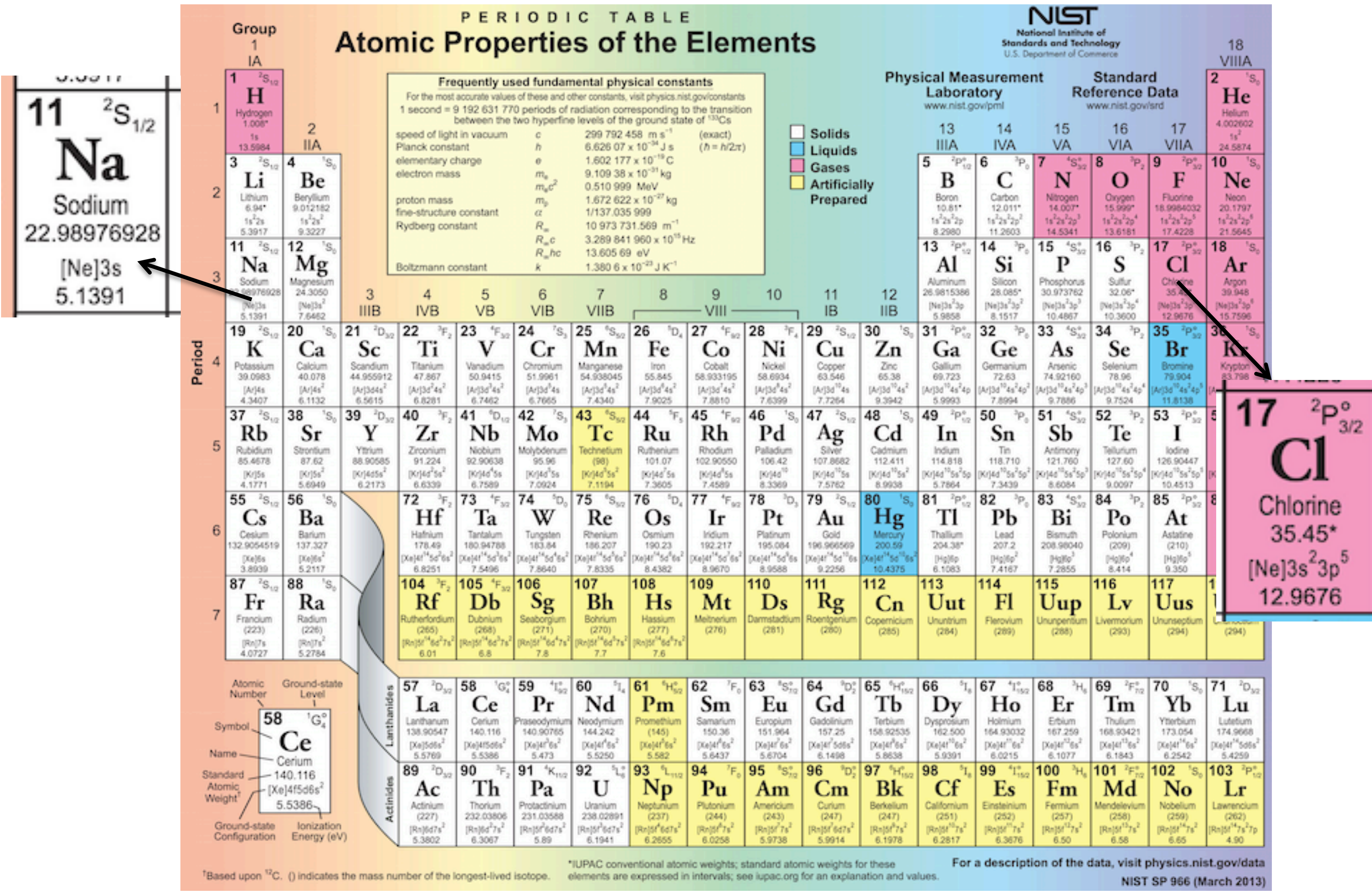
- Stable electron configurations = valence electrons shells are completely filled (e.g. inert gasses)

Argon	Ar	18	$1s^2 2s^2 2p^6 3s^2 3p^6$

SURVEY OF ELEMENTS

- **Most elements: Electron configuration not stable.**

Element	Atomic #	Electron configuration	
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	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4^6$	(stable)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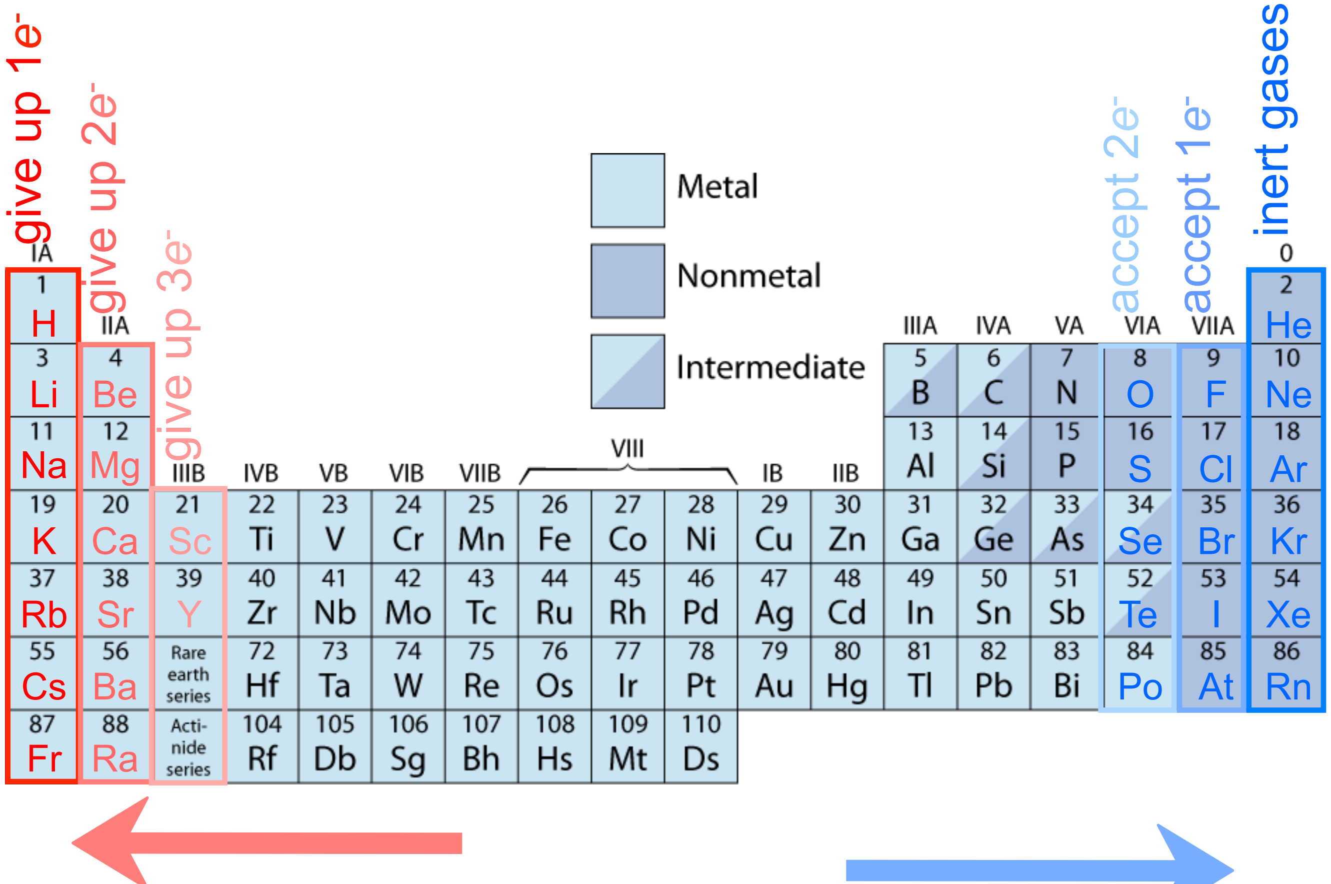
www.nist.gov/srd
Solids
Liquids
Gases
Artificially Prepared
Group
Period
Lanthanides
Actinides
11 $^2S_{1/2}$
Na
Sodium
22.98976928
[Ne]3s
5.1391
17 $^2P^o_{3/2}$
Cl
Chlorine
35.45*
$[Ne]3s^23p^5$
12.9676
For a description of the data, visit physics.nist.gov/data
NIST SP 966 (March 2013)

The Periodic Table

- Columns: Similar Valence Structure



Electropositive elements:
Readily give up electrons
to become + ions.

Electronegative elements:
Readily acquire electrons
to become - ions.

e.g. Mg $1s^2\ 2s^2\ 2p^6\ 3s^2 \rightarrow Mg^{2+}\ 1s^2\ 2s^2\ 2p^6$

Electronegativity

- Ranges from 0.9 to 4.1,
- Large values: tendency to acquire electrons.

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII	VIII	VIII	IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
H 2.1																	He –
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.1	O 3.5	F 4.1	Ne –
Na 1.0	Mg 1.3											Al 1.5	Si 1.8	P 2.1	S 2.4	Cl 2.9	Ar –
K 0.9	Ca 1.1	Sc 1.2	Ti 1.3	V 1.5	Cr 1.6	Mn 1.6	Fe 1.7	Co 1.7	Ni 1.8	Cu 1.8	Zn 1.7	Ga 1.8	Ge 2.0	As 2.2	Se 2.5	Br 2.8	Kr –
Rb 0.9	Sr 1.0	Y 1.1	Zr 1.2	Nb 1.3	Mo 1.3	Tc 1.4	Ru 1.4	Rh 1.5	Pd 1.4	Ag 1.4	Cd 1.5	In 1.5	Sn 1.7	Sb 1.8	Te 2.0	I 2.2	Xe –
Cs 0.9	Ba 0.9	La 1.1	Hf 1.2	Ta 1.4	W 1.4	Re 1.5	Os 1.5	Ir 1.6	Pt 1.5	Au 1.4	Hg 1.5	Tl 1.5	Pb 1.6	Bi 1.7	Po 1.8	At 2.0	Rn –
Fr 0.9	Ra 0.9	Ac 1.0															

Lanthanides: 1.0-1.2
Actinides: 1.0-1.2

Smaller electronegativity ← → Larger electronegativity

INTERATOMIC BONDING

Atomic Bonds

Primary interatomic bonds

- depends on the electron structures of the atoms
- Seeks stable electron structures (by filling the outermost electron shell)

Ionic bonding

Covalent bonding

Metallic bonding

Secondary, van der Waals, or physical bonds

1. IONIC BONDING

Ionic bond – metal + nonmetal

metal → donates electrons

nonmetal → accepts electrons

Dissimilar electronegativities

ex: MgO   Mg $1s^2\ 2s^2\ 2p^6\ 3s^2$ O $1s^2\ 2s^2\ 2p^4$

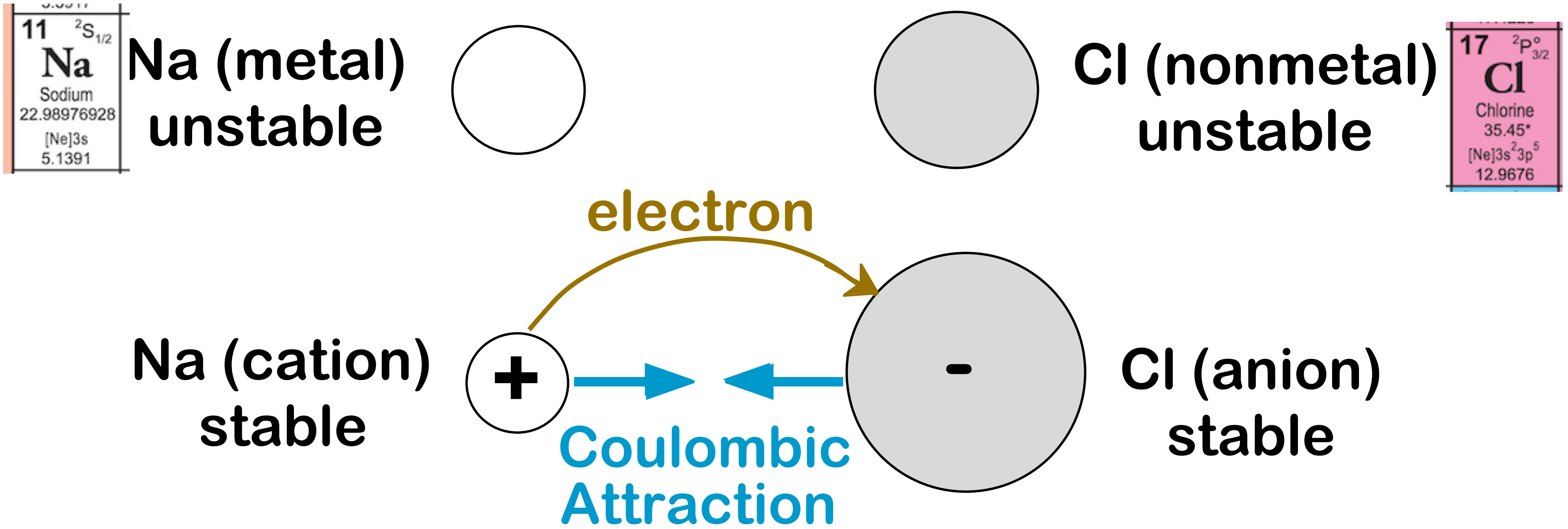
[Ne] $3s^2$

Mg^{2+} $1s^2\ 2s^2\ 2p^6$ O^{2-} $1s^2\ 2s^2\ 2p^6$

[Ne]   [Ne]

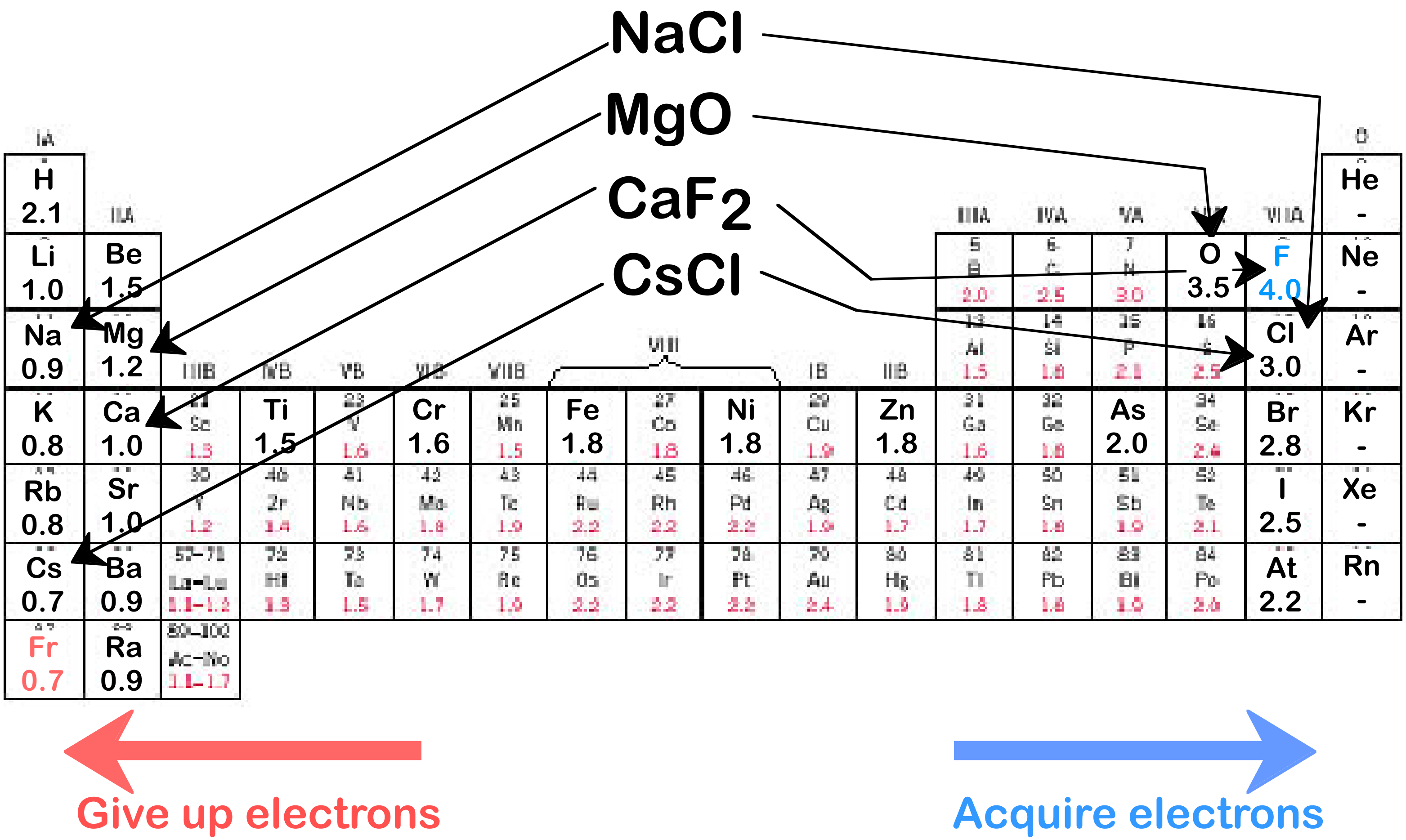
1. IONIC BONDING

- Occurs between + and - ions.
- Requires electron transfer.
- Example: NaCl



EXAMPLES: IONIC BONDING

- **Predominant bonding in Ceramics**



Section 2.6

Ionic materials (materials with predominate ionic bonding):

- Most ceramic materials have ionic bonding
- Bonding energy is relatively large ➔ High melting temperature
- Ionic materials are hard and brittle
- Electrically and thermally insulative
- Covalent bonding is nondirectional

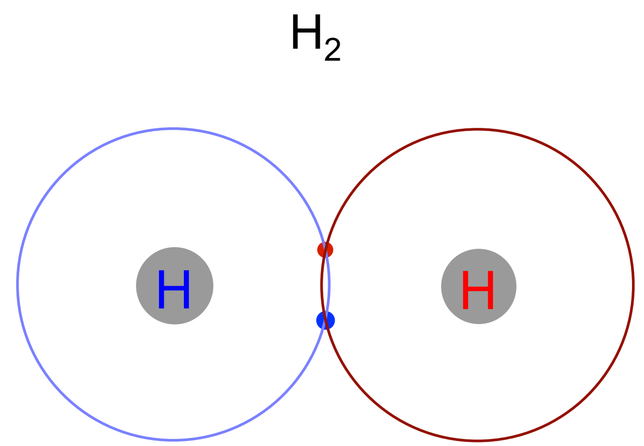
2. Covalent Bonding

- **Requires shared electrons**
- similar electronegativity ∴ share electrons

Example: H_2

Each H: has 1 valence e^-,
needs 1 more

Electronegativities
are the same.



• shared 1*s* electron from 1st hydrogen atom

• shared 1*s* electron from 2nd hydrogen atom

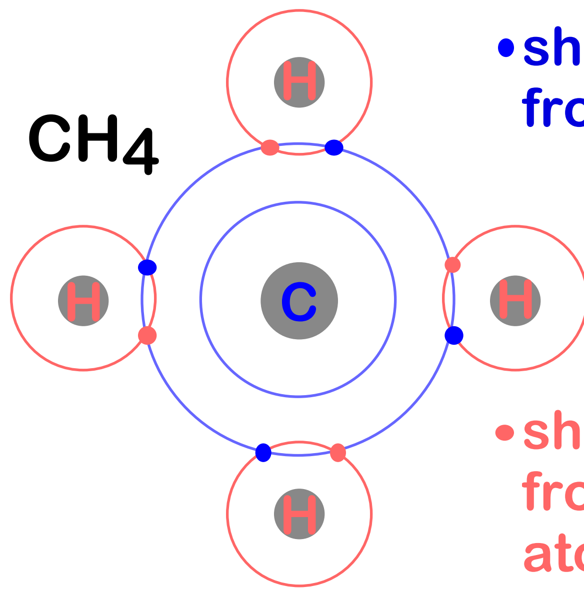
2. COVALENT BONDING

- Requires shared electrons
- Example: CH4

C: has 4 valence e,
needs 4 more

H: has 1 valence e,
needs 1 more

Electronegativities
are comparable.



2. COVALENT BONDING

- Available in
  - Most nonmetallic elemental molecules (H_2, Cl_2, F_2, etc)
  - CH_4, H_2O, HF, etc
  - Elemental solids such as diamond, silicon, germanium
  - Polymers

- Bonding may be weak or strong

- Ionic bonding is directional

It should be noted that partially ionic and partially covalent bonding are possible

3. METALLIC BONDING

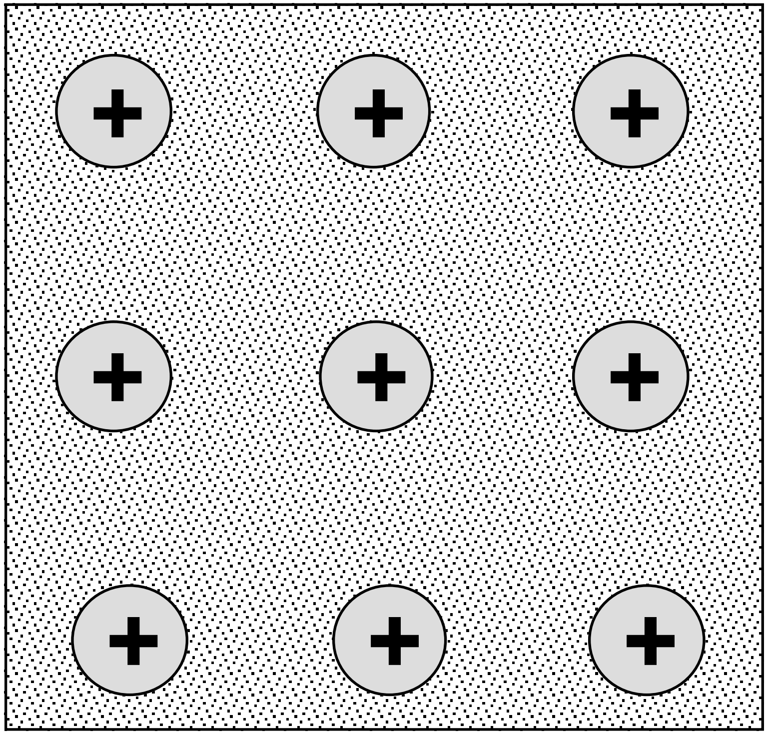
- ✓ Primary bond for metals and their alloys
- ✓ Arises from a sea of donated valence electrons

① Metallic elements have 1, 2, or 3 valence electrons ➔ Electron clouds (negative charge)

+

② Non valence electrons and atomic nuclei ➔ ions cores (positive charge)

= forms Metallic bonding

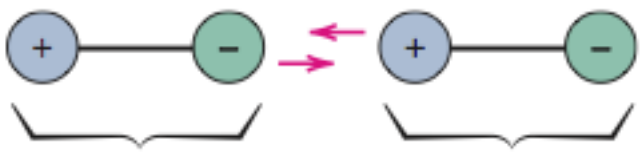


3. METALLIC BONDING

- Primary bond for metals
- Good electric and thermal conductivities (because of the free electrons)
- Bonding may be weak or strong
- Metallic bonding is nondirectional

Secondary Bonding or van der Waals Bonding

- Secondary bonding arise from interaction between atomic or molecular **dipoles**



Dipole is a pair of equal yet opposite electrical charges that are separated by a small distance.

- Weak bonding (10 kJ/mol)

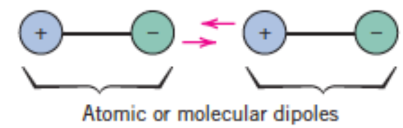
- Can exist between all atoms or molecules

- *Fluctuating induced dipole bond, polar molecule- induced dipole bond, permanent dipole bond, and hydrogen bond* ***(see section 2.7)***

Atomic Bonds

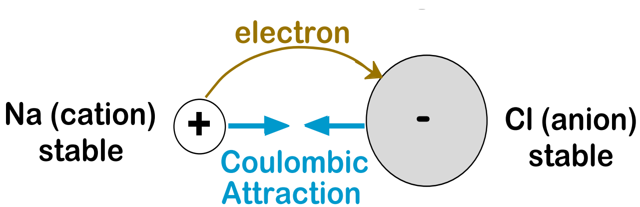
Primary interatomic bonds

Secondary, van der Waals, or physical bonds



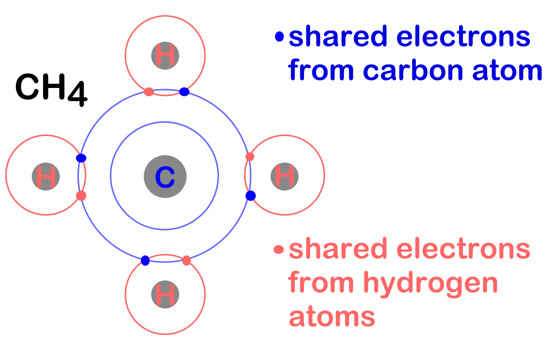
Ionic bonding

Atoms give up their valence electrons to other atoms



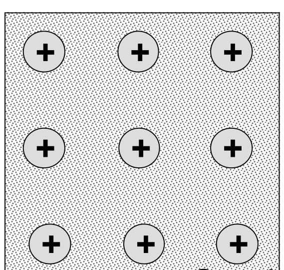
Covalent bonding

share electrons between adjacent atoms



Metallic bonding

Arises from a sea of donated valence electrons



SUMMARY: BONDING

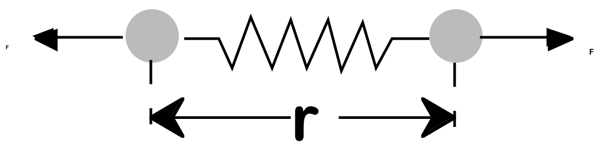
Type	Bond Energy	Comments
Ionic	Large!	Nondirectional (ceramics)
Covalent	Variable large-Diamond small-Bismuth	Directional semiconductors, ceramics polymer chains)
Metallic	Variable large-Tungsten small-Mercury	Nondirectional (metals)
Secondary	smallest	Directional inter-chain (polymer) inter-molecular

Section 2.6

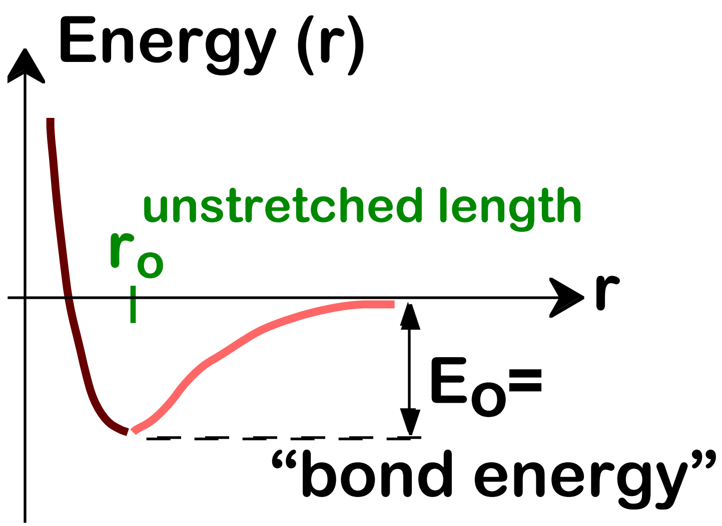
Relationships between bonding and some physical properties

PROPERTIES FROM BONDING: T_M

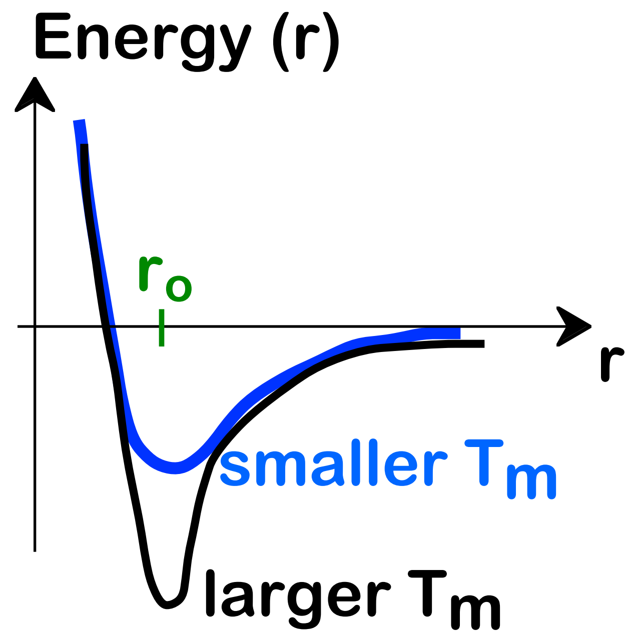
- **Bond length**, r



- **Bond energy**, E_o



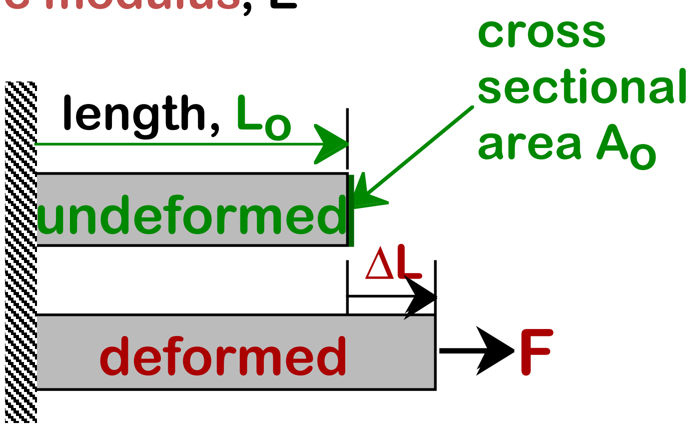
- **Melting Temperature**, T_m



T_m is larger if E_o is larger.

PROPERTIES FROM BONDING: E

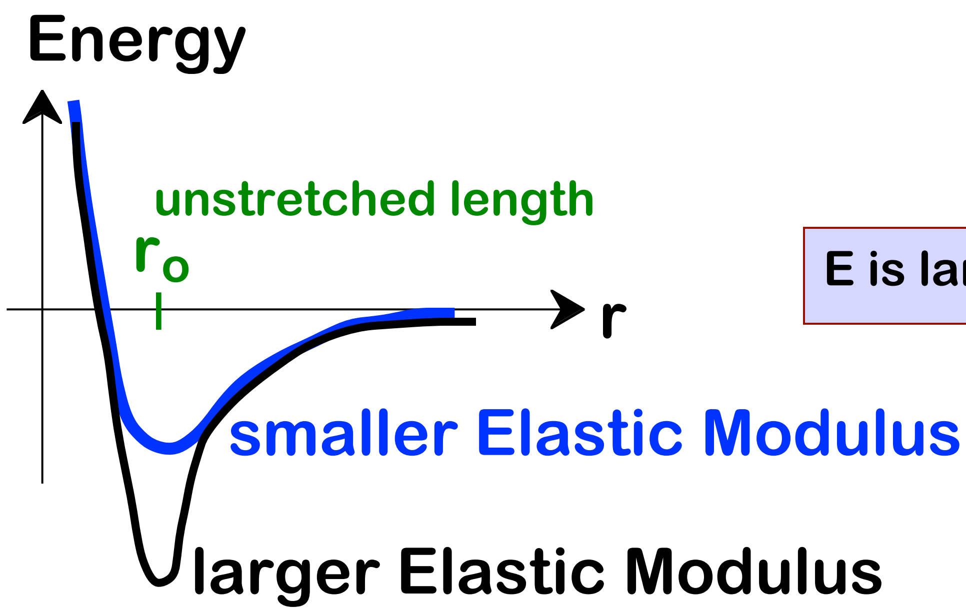
- Elastic modulus, E



Elastic modulus

$$\frac{F}{A_o} = E\,\frac{\Delta L}{L_o}$$

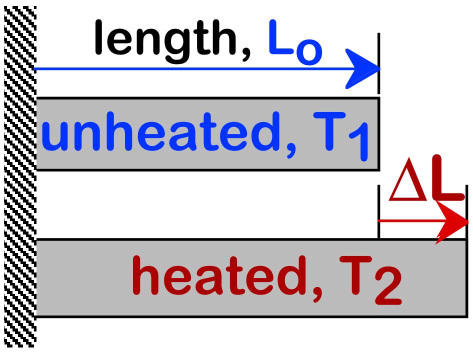
- E ~ curvature at r_o



E is larger if E_o is larger.

PROPERTIES FROM BONDING: α

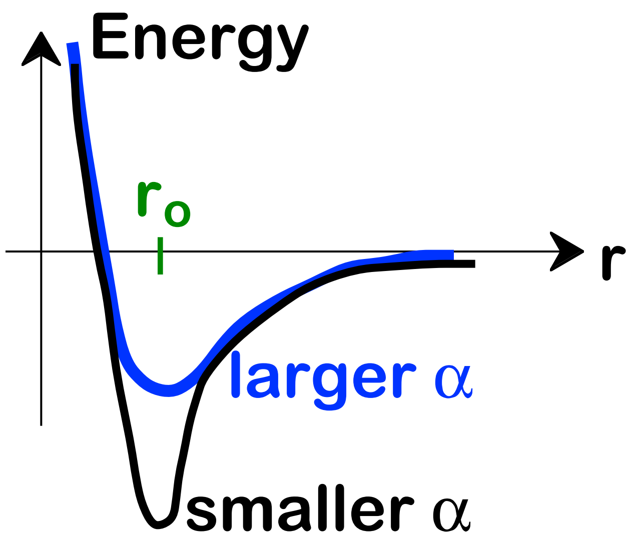
- **Coefficient of thermal expansion**, α



coeff. thermal expansion

$$\frac{\Delta L}{L_o} = \alpha\,(T_2 - T_1)$$

- α ~ symmetry at r_o



α is larger if E_o is smaller.

SUMMARY: PRIMARY BONDS

Ceramics

(Ionic & covalent bonding):

Large bond energy
large T_m
large E
small α

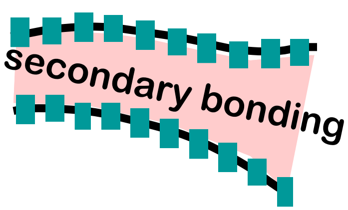
Metals

(Metallic bonding):

Variable bond energy
moderate T_m
moderate E
moderate α

Polymers

(Covalent & Secondary):



Directional Properties
Secondary bonding dominates
small T
small E
large α

Chapter 2: Summary

1) **Atomic structure and electron configurations**

2) **Interatomic bonding**

(primary & secondary, van der Waals, bonding)