

Classes of Materials

	POLYMERS	CERAMICS	METALS
DUCTILITY	Varies	Poor	Good
CONDUCTIVITY (ELECTRICAL & THERMAL)	Low	Low	High
HARDNESS/STRENGTH	Low – medium	High	Medium– high
CORROSION RESISTANCE	Fair – good	Good	Fair – poor
STIFFNESS	Low	High	Fair
FRACTURE TOUGHNESS	Low – Medium	Low	High
MACHINABILITY	Good	Low	High

Why study bonding?

- Because the **properties of materials** (*strength, hardness, conductivity, etc..*) are determined by the manner in which atoms are connected.

What determines the nature of the chemical bond between atoms?

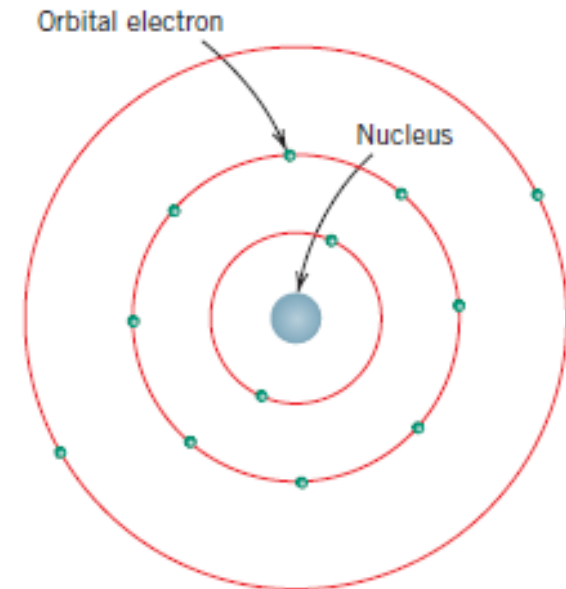
- Electronic structure (distribution of electrons in atomic orbitals)
- Number of electrons and protons (tendency for an atom to attract an electron)

Atomic Structure

□ Bohr model of the atom: (1913)

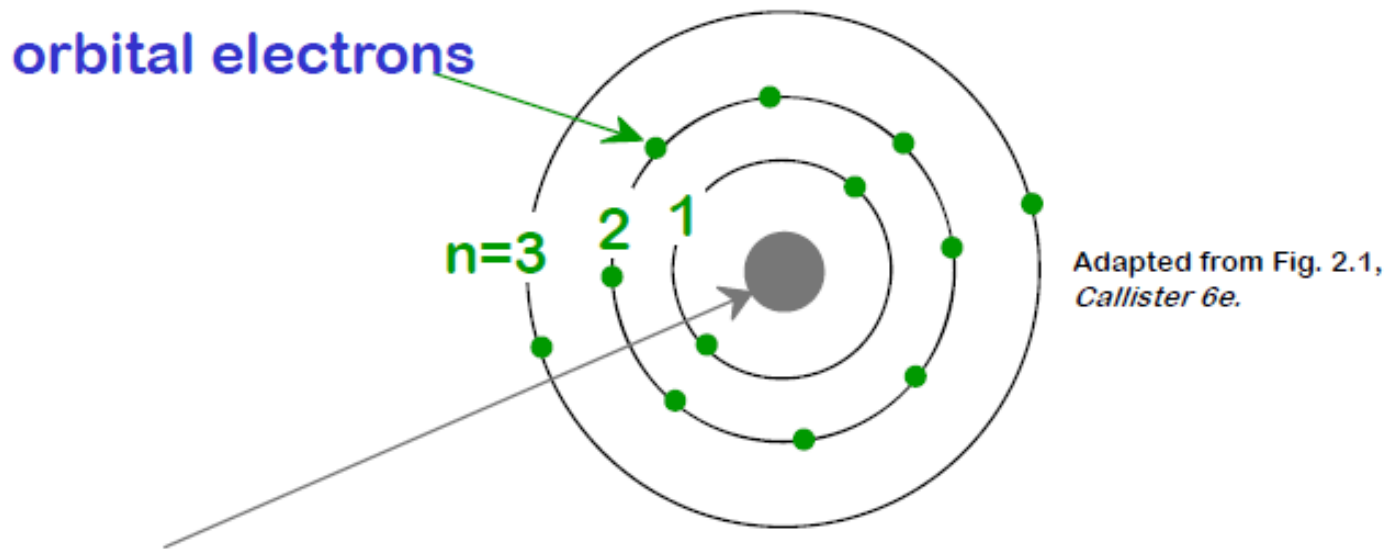
– Bohr atomic model

- electrons revolve around nucleus in discrete orbitals



Based on earlier work of Rutherford and his own from spectral emission studies

BOHR ATOM



Adapted from Fig. 2.1,
Callister 6e.

Nucleus: $Z = \#$ protons

= 1 for hydrogen to 94 for plutonium

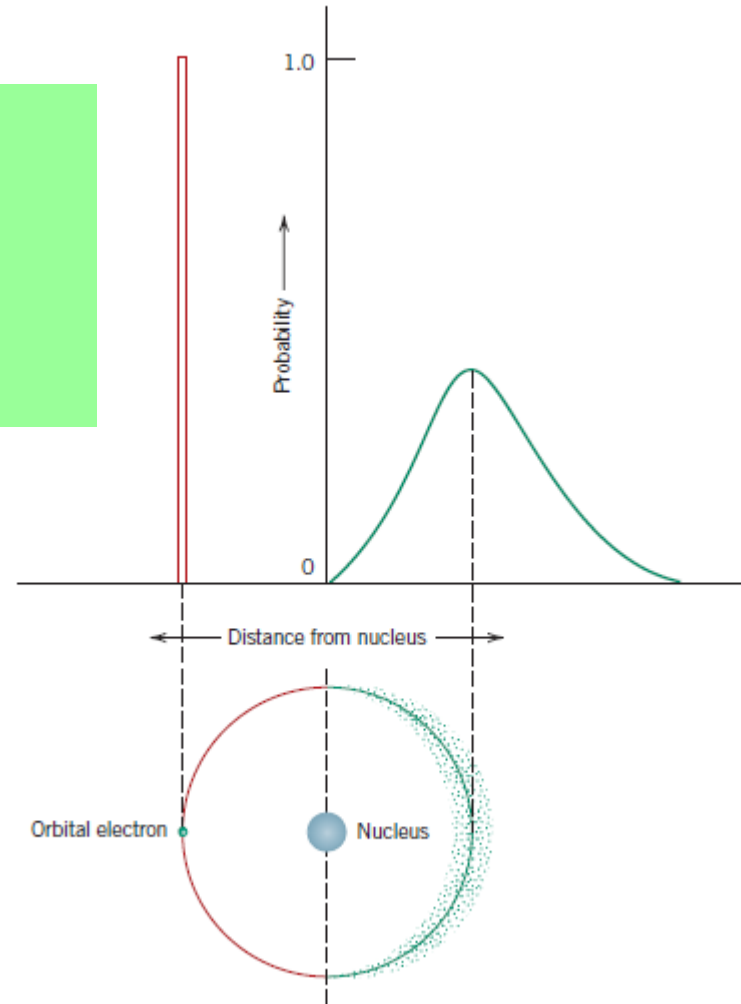
$N = \#$ neutrons

Atomic mass $A \approx Z + N$

Bohr vs. Quantum-Mechanical Model: (1927)

- ❑ Wave-mechanical atomic model
- Position of electron is imprecisely known; only a probability distribution.
- Electron exhibits both particle and wave characteristics

*Schroedinger, Heisenburg, Planck and others developed this model (**wave mechanics**), which allows a more precise description of the atom.*



Increasing Electronegativity →

s-block
 1 New Designation
 IA Original Designation

s-block
 18
 VIIIA

		Non-Metals											
		Atomic #											
		Symbol											
		Atomic Mass											
		<i>p</i> -block											
		<i>d</i> -block											
		Transition Metals											
		<i>f</i> -block											
		Metals											

	1	H	2																	2	He
		1.0094																		4.00260	
		<i>s</i> -block																			
	2	Li	Be											B	C	N	O	F	Ne		
		6.941	9.0122											10.81	12.011	14.007	15.999	18.998	20.179		
	3	Na	Mg	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18		
		22.990	24.305	IIIB	IVB	VB	VIB	VII B	VIII B	VIII B	IB	IIB		Al	Si	P	S	Cl	Ar		
														26.982	28.086	30.974	32.06	35.453	39.948		
	4	K	Ca	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36		
		39.098	40.08	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
				44.956	47.88	50.942	51.996	54.938	55.847	58.933	58.69	63.546	65.39	69.72	72.59	74.922	78.96	79.904	83.80		
	5	Rb	Sr	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54		
		85.468	87.62	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
				88.906	91.224	92.906	95.94	(98)	101.07	102.91	106.42	107.87	112.41	114.82	118.71	121.75	127.60	126.91	131.29		
	6	Cs	Ba	57	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86		
		132.91	137.33	to 71	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn		
					178.49	180.95	183.85	186.21	190.2	192.22	195.08	196.97	200.59	204.38	207.2	208.98	(209)	(210)	(222)		
	7	Fr	Ra	89	104	105	106	107	108	109	110								(Mass Numbers in Parentheses are from the most stable of common isotopes.)		
		(223)	(226.03)	to 103	Unq	Unp	Unh	Uns	Uno	Une	Uun								Phases Solid Liquid Gas		
					(261)	(262)	(263)	(262)	(265)	(266)	(267)										

	Rare Earth Elements	<i>d</i> -block										<i>f</i> -block									
	Lanthanide Series	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71					
		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu					
		138.91	140.12	140.91	144.24	(145)	150.36	151.96	157.25	158.93	162.50	164.93	167.26	168.93	173.04	174.97					
	Actinide Series	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103					
		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr					
		227.03	232.04	231.04	238.03	237.05	(244)	(243)	(247)	(247)	(251)	(252)	(257)	(258)	(259)	(260)					

- <http://www.webelements.com>

Electronegativity - each kind of atom has a certain attraction for the electrons involved in a chemical bond. This "electronattracting" power of each atom can be listed numerically on an electronegativity scale.

Electronegativity Values of Selected Elements

Metallic Elements			Nonmetallic Elements			
Li (1.0)	Be (1.5)		C (2.5)	N (3.0)	O (3.5)	F (4.0)
Na (1.0)	Mg (1.2)	Al (1.5)		P (2.1)	S (2.5)	Cl (3.0)
K (0.9)	Ca (1.0)	Sc (1.3)			Se (2.4)	Br (2.8)

❖ *Electronegativity was originally worked out by Linus Pauling in 1939*

The Periodic Table

- **Columns:** Similar Valence Structure

Give up 1e		Give up 2e		Give up 3e										Accept 2e					Accept 1e	Inert gases
IA	IIA	IIIB	IVB	VB	VIB	VIIIB	VIII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA	0		
1 H 1.0080	4 Be 9.0122											5 B 10.811	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.180			
11 Na 22.990	12 Mg 24.305											13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.064	17 Cl 35.453	18 Ar 39.948			
19 K 39.098	20 Ca 40.08	21 Sc 44.956	22 Ti 47.87	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.845	27 Co 58.933	28 Ni 58.69	29 Cu 63.54	30 Zn 65.41	31 Ga 69.72	32 Ge 72.64	33 As 74.922	34 Se 78.96	35 Br 79.904	36 Kr 83.80			
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.4	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.76	52 Te 127.60	53 I 126.90	54 Xe 131.30			
55 Cs 132.91	56 Ba 137.34	Rare earth series	72 Hf 178.49	73 Ta 180.95	74 W 183.84	75 Re 186.2	76 Os 190.23	77 Ir 192.2	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.19	83 Bi 208.98	84 Po (209)	85 At (210)	86 Rn (222)			
87 Fr (223)	88 Ra (226)	Actinide series	104 Rf (261)	105 Db (262)	106 Sg (266)	107 Bh (264)	108 Hs (277)	109 Mt (268)	110 Ds (281)											

Key

- Atomic number
- Symbol
- Atomic weight

- Metal
- Nonmetal
- Intermediate



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



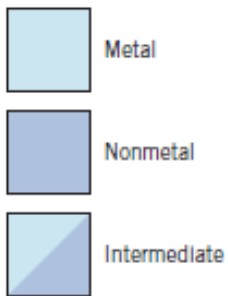
Electronegative elements:
Readily acquire electrons
to become - ions.

Electronegativity

- Ranges from 0.7 to 4.0,
- Large values: tendency to acquire electrons.

IA												0						
1 H 1.0080												2 He 4.0026						
IIA												III A	IV A	VA	VIA	VII A	VIII A	
3 Li 6.941	4 Be 9.0122											5 B 10.811	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.180	
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87 Fr (223)	88 Ra (226)	Acti-nide series	104 Rf (261)	105 Db (262)	106 Sg (266)	107 Bh (264)	108 Hs (277)	109 Mt (268)	110 Ds (281)									

Key
 29 ← Atomic number
 Cu ← Symbol
 63.54 ← Atomic weight



←
 Smaller electronegativity

→
 Larger electronegativity

Electronegativity

- ✓ **High electronegativity** → strong tendency to accept an electron (i.e., Group VIIA: F, Cl)
- ✓ **Low electronegativity** (called “electropositive”) → strong tendency to give up an electron, i.e., Group IA: Li, Na, K)

The difference in electronegativity between two atoms determines the resulting electron distribution and the type of bond

Density, Atomic # & Wt, Mole & Avogadro's

- **Density**

- g/cm³ (most solids range ~ 1 - 23 g/cm³)

- **Atomic number** = number of protons (Z)

- **Atomic weight (A)**

- g/mole

A = number protons (Z) + neutrons (N)

= Z+N

- Mole = number of particles 1 amu/atom or molecule = 1 g/mol

In one **mole** of a substance there are 6.023×10^{23} (Avogadro's number) atoms or molecules

Review Problems

- How many atoms in 6 grams of carbon?

$$\begin{aligned} \text{Number of moles} &= \frac{\text{Mass}}{\text{Mwt}} \\ &= \frac{6}{12} = 0.5 \end{aligned}$$

$$\text{Number of atoms} = 0.5 * 6.023 * 10^{23}$$

- **Calculate the volume of 1 mole of Au.**

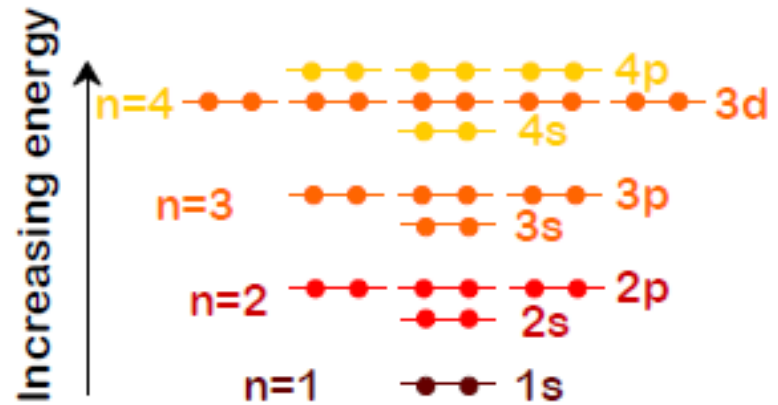
$$\text{mass} = \text{of moles} * \text{Mwt} = 1 * 196.97$$

$$\text{Volume} = \frac{\text{Mass}}{\rho_{\text{Au}}} = \frac{196.96 \text{ (g)}}{19.3 \left(\frac{\text{g}}{\text{mL}}\right)}$$

Electron energy state

Electrons

- have discrete **energy states**
- tend to occupy lowest available energy state.

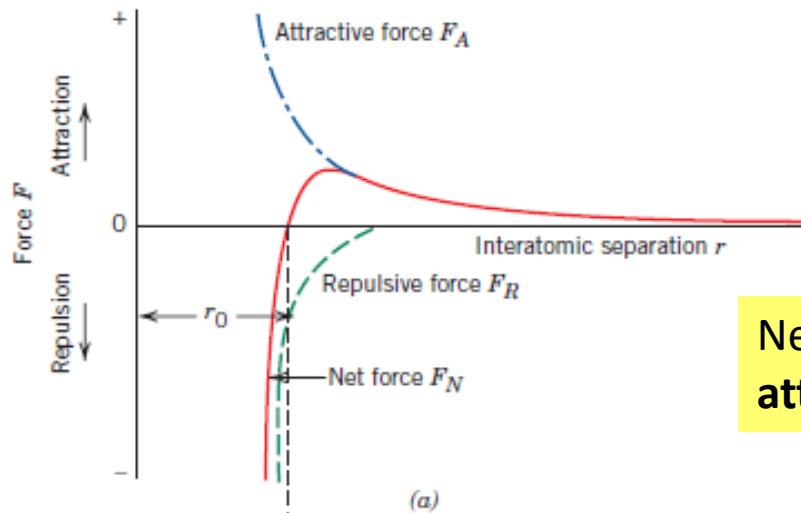


Stable electron configurations...

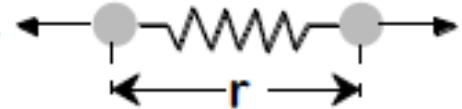
- have complete s and p subshells

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

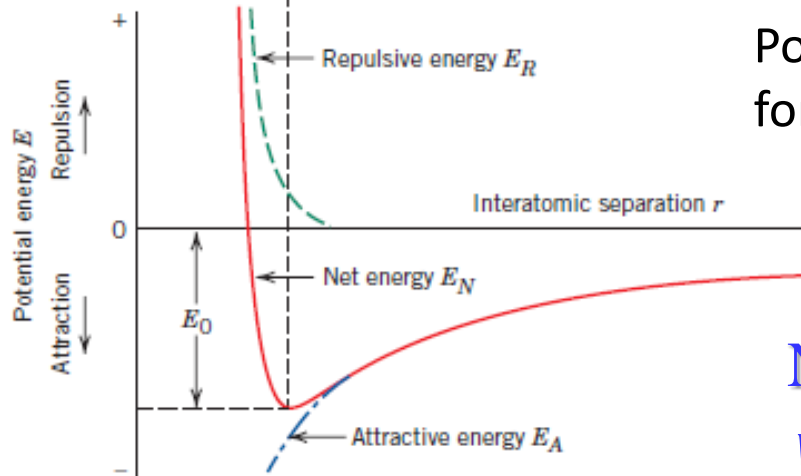
Bonding Forces and Energies



Bond length, r



Net force is given by the **sum** of an **attractive** force and a **repulsive** force



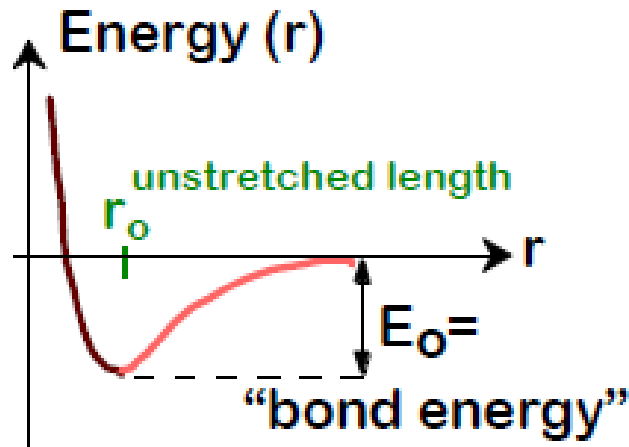
Potential is given by the integral of the net force curve with respect to distance:

$$E = \int F \cdot dr$$

Note: equilibrium separation occurs where the net force = 0

Bonding energy: *Minimum of the potential vs. distance curve.*

- Indicates how much energy must be supplied to completely disassociate the two atoms
- Depth of the potential well indicates bonding strength
 - Deep well === strongly bounded
 - Shallow well === weakly bounded



Bound energy

□ The higher the bond energy

- Higher melting temperature
- Solid material

□ State as function of bonding energy

- Solid: high bonding energy
- Liquid: Moderate BE
- Gas: Low BE