M. Sc. Bionics Engineering

Università di Pisa — Sant'Anna Scuola Universitaria Superiore Pisa — IMT Scuola Alti Studi Lucca

Advanced Materials for Bionics

Lecture 2: Materials Structure 1

Bonding

Prof. Francesco Greco

AY 2024-25

L2 - 27.09.2024

COURSE SECTIONS

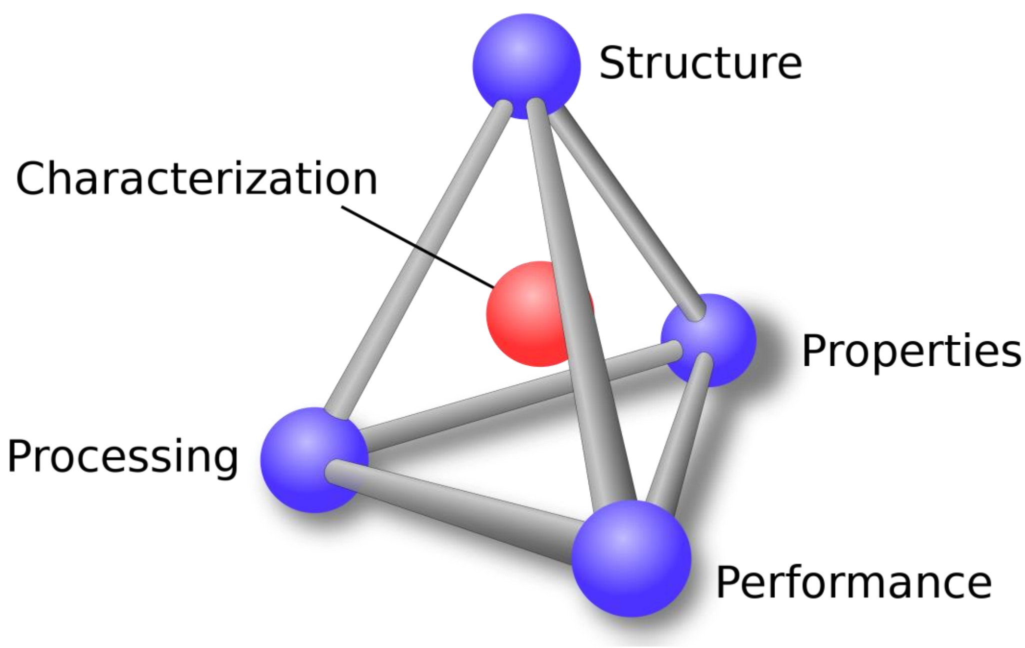
Section 1:
Refresh of Basics Materials Science
(Lectures ≈ 2 - 10)

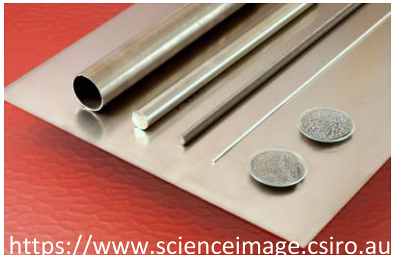
- Materials structure & properties
- Materials classes

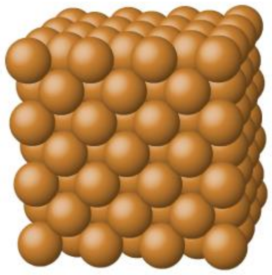
Section 2:
Advanced Concepts
+ Technology &Bionics applications
(Lectures ≈11 - 18)

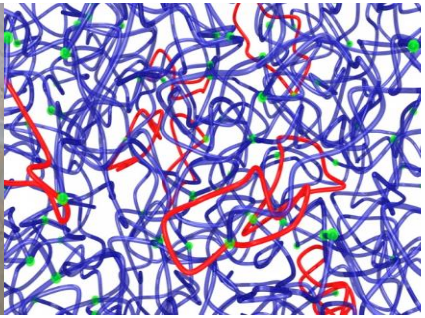
- Biological materials science
- Bioinspiration biomimetics
- Smart materials
- Nanotechnology
- Fab/patterning
- Additive Manufacturing
- Robotics
- Bioelectronics
- Biomedicine

MATERIALS STRUCTURE









QUESTIONS

- What characteristics of atoms/molecules promote interatomic/intermolecular bonding?
- What types of interatomic/intermolecular bonds exist ?
- What properties of materials depend on the magnitude of interatomic/intermolecular bonds ?

Metal

Nonmetal

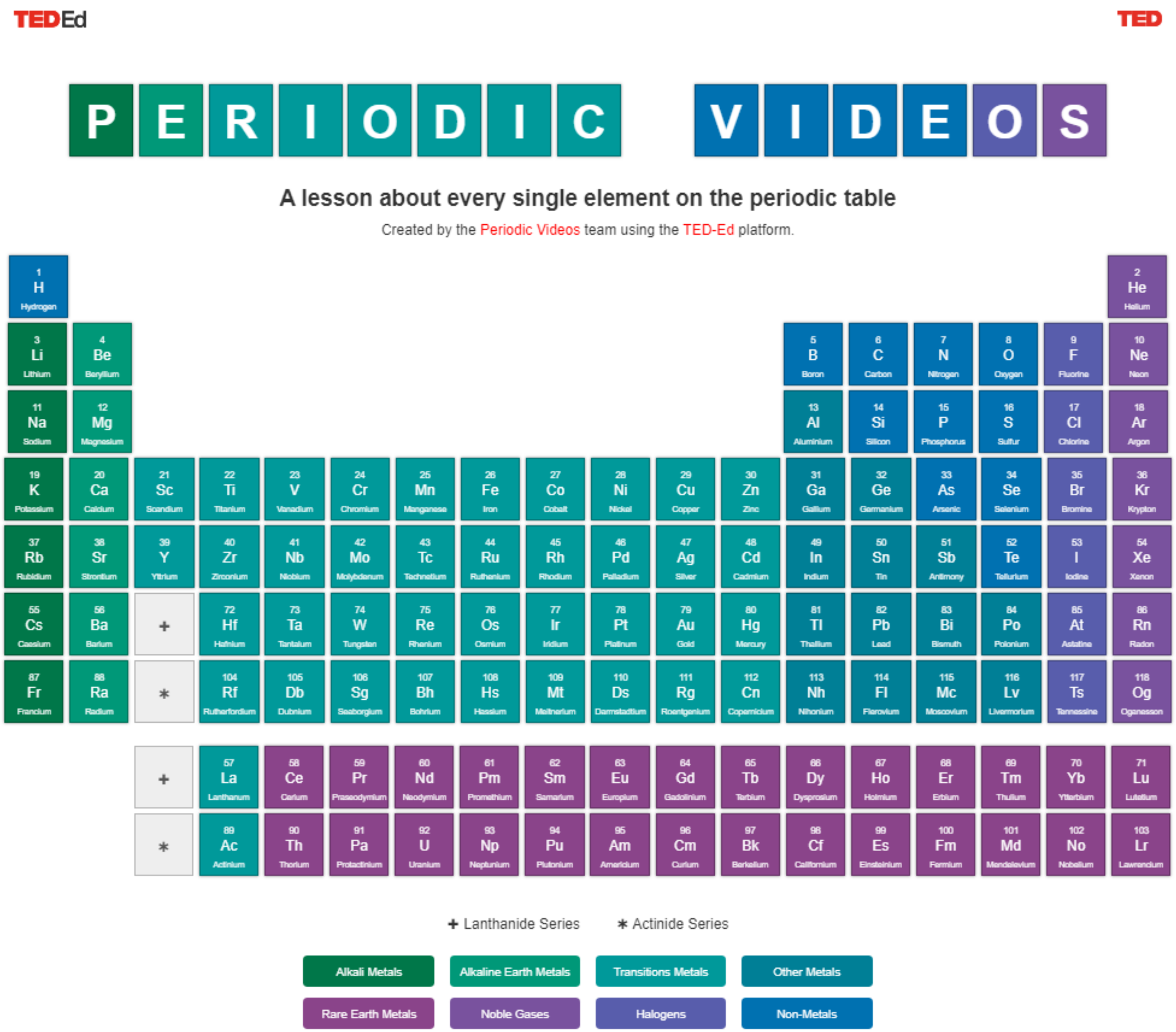
Intermediate

Key: 29 ← Atomic number; Cu ← Symbol; 63.55 ← Atomic weight

IA (1)	IIA (2)	IIIB (3)	IVB (4)	VB (5)	VIB (6)	VIIB (7)	VIII (8)	VIII (9)	VIII (10)	IB (11)	IIB (12)	IIIA (13)	IVA (14)	VA (15)	VIA (16)	VIIA (17)	0 (18)
1 H 1.0080																	2 He 4.0026
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
11 Na 22.990	12 Mg 24.305											13 Al 26.982	14 Si 28.085	15 P 30.974	16 S 32.064	17 Cl 35.453	18 Ar 39.948
19 K 39.098	20 Ca 40.078	21 Sc 44.956	22 Ti 47.867	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 63.55	30 Zn 65.38	31 Ga 69.72	32 Ge 72.63	33 As 74.922	34 Se 78.97	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 95.95	43 Tc (98)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.42	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 131.29
55 Cs 132.91	56 Ba 137.33	Rare earth series	72 Hf 178.49	73 Ta 180.95	74 W 183.84	75 Re 186.21	76 Os 190.23	77 Ir 192.22	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.2	83 Bi 208.98	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	Acti-nide series	104 Rf (267)	105 Db (268)	106 Sg (269)	107 Bh (270)	108 Hs (269)	109 Mt (278)	110 Ds (281)	111 Rg (280)	112 Cn (285)	113 Uut (286)	114 Fl (289)	115 UUp (289)	116 Lv (293)	117 Uus (294)	118 Uuo (294)

Rare earth series	57 La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.96	64 Gd 157.25	65 Tb 158.92	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97
Actinide series	89 Ac (227)	90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)

[TED-Ed and Periodic Videos](#)

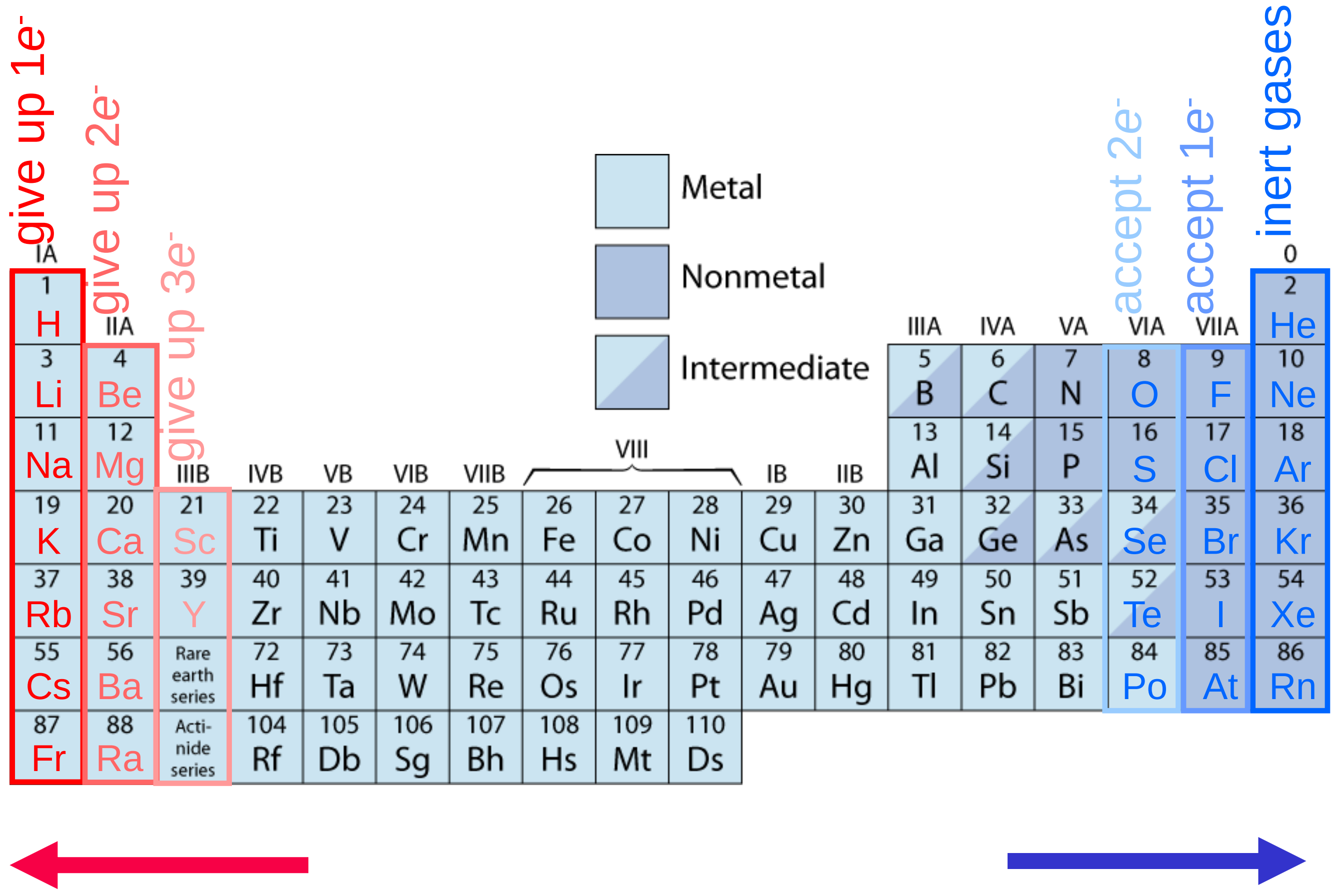


L2.1

Interatomic Bonds

The Periodic Table

Elements in each column: Similar valence electron structure



Electropositive elements:
Readily give up electrons to become + ions

Electronegative elements:
Readily acquire electrons to become - ions

ELECTRONEGATIVITY

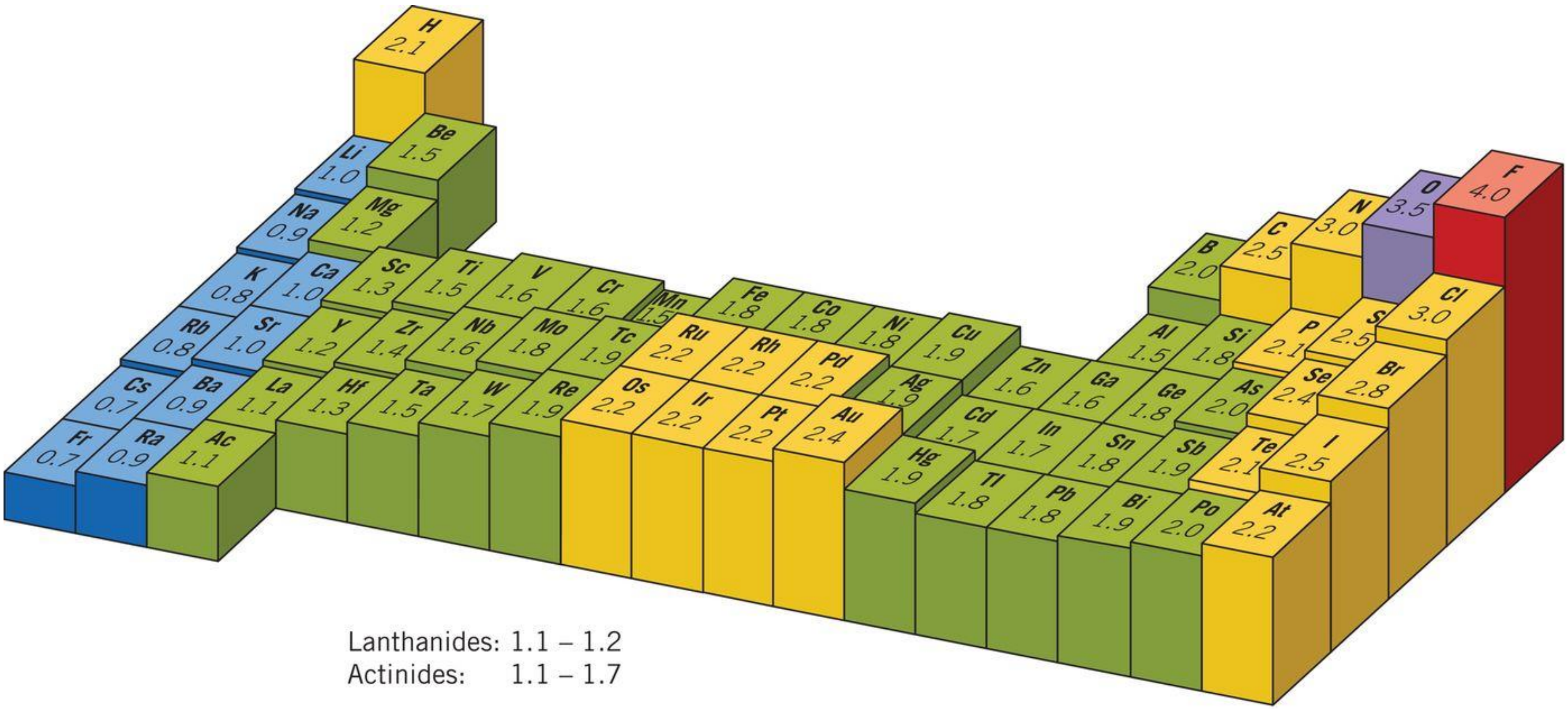
- Ranges from 0.7 to 4.0,
- Large values: tendency to acquire electrons.

IA	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 3.0	O 3.5	F 4.0	Ne –
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ar –
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr –
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe –
Cs 0.7	Ba 0.9	La–Lu 1.1–1.2	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 –
Fr 0.7	Ra 0.9	Ac–No 1.1–1.7															

Smaller electronegativity

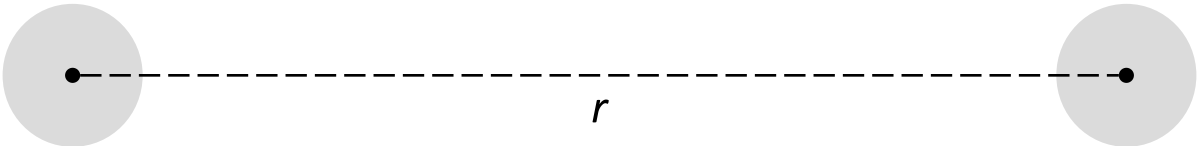
Larger electronegativity

ELECTRONEGATIVITY

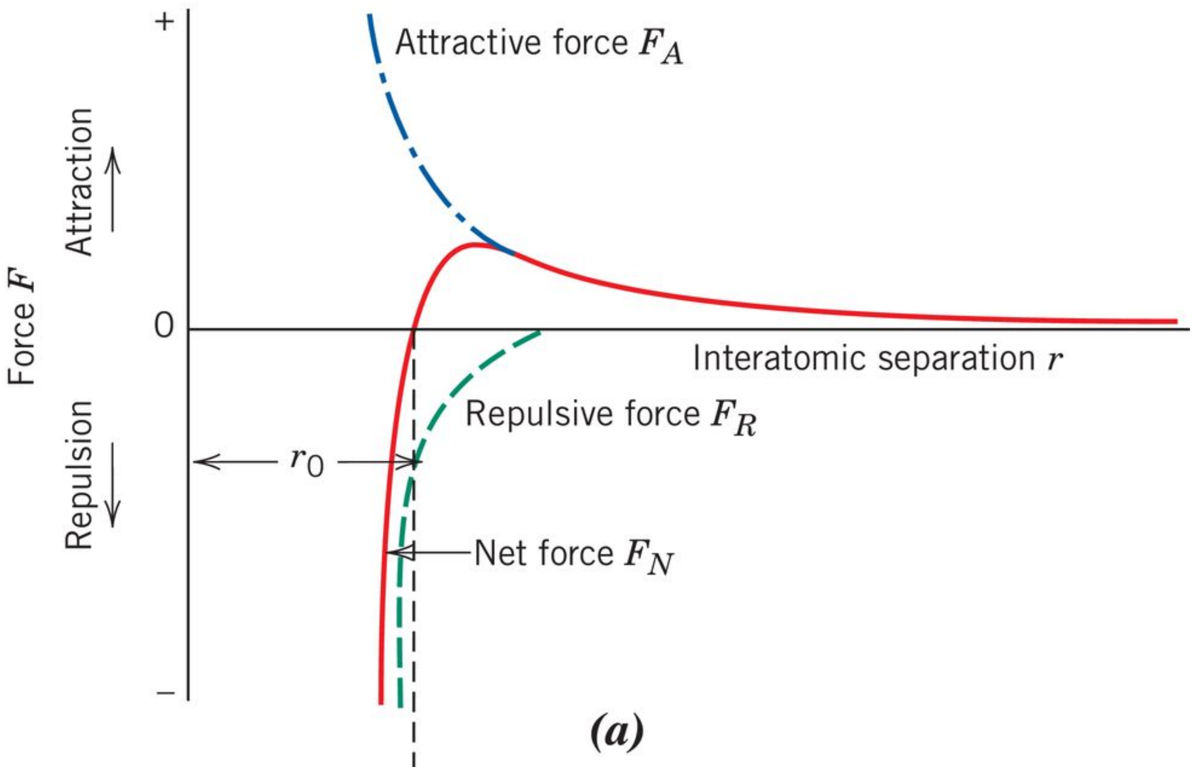


From J. E. Brady and F. Senese, *Chemistry: Matter and Its Changes*, 4th edition, 2004. This material is reproduced with permission of John Wiley & Sons, Inc.

Bonding Force



$$F_N = F_A + F_R$$

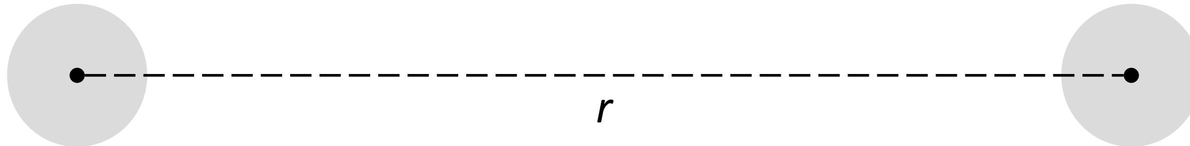


r_0

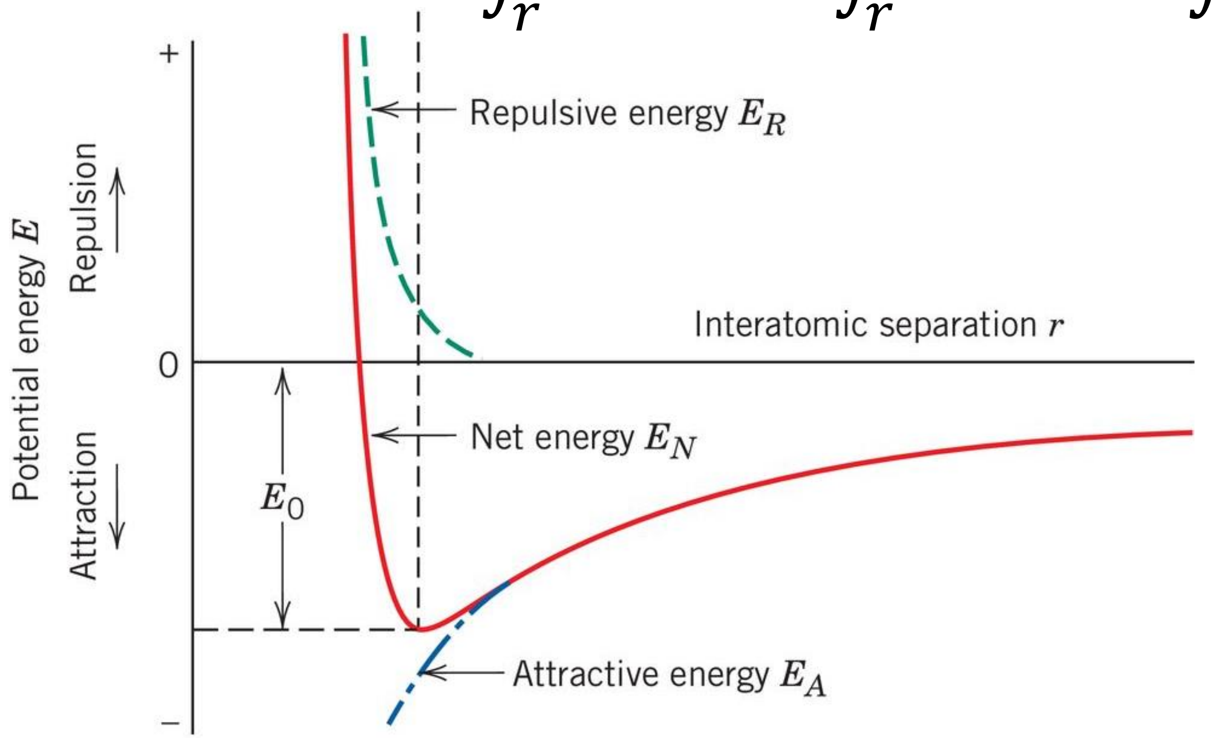
equilibrium distance

$$F_A + F_R = 0$$

Bonding Energy



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



E_0

Bonding (Net) Energy

Bonding Energy and Materials

2 atoms $\longrightarrow E_0$ **bonding energy**

IN APPENDIX
Cohesive energy

In solids? Many atoms, much more complex!

But analogous E_0 can be defined for each atom in a solid

$E(r), E_0$ depend on type of **interatomic bond**

- **primary**
  - ionic
  - covalent
  - metallic
- **secondary**
  - Hydrogen
  - Van der Waals
  - …

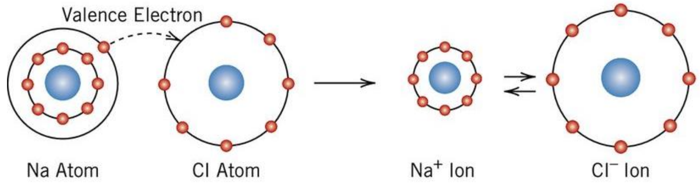
Many properties of materials depend on $E(r), E_0$

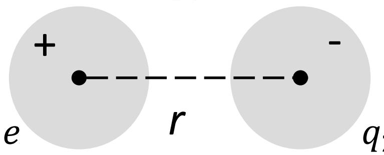
- phase (gas, liquid, solid)
- melting temperature T_m
- Elastic modulus
- thermal exp. coeff.
- …

L2.1.1

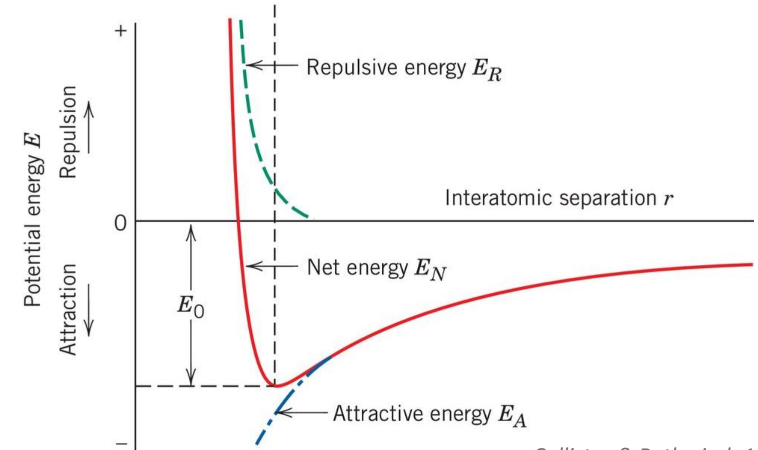
PRIMARY INTERATOMIC BONDS

IONIC BONDING





$q_1 = Z_1 e$ $\qquad$ $q_2 = Z_2 e$



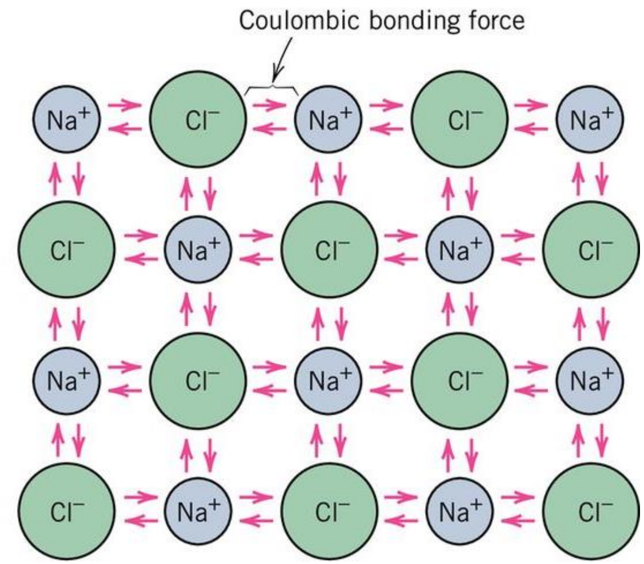
Callister & Rethwisch 10e

$$E_A = -\frac{A}{r} \qquad A = \frac{(|Z_1|e)(|Z_2|e)}{4\pi\varepsilon_0}$$ Coulomb's law

$$E_R = \frac{B}{r^n}$$ typ. $n \approx 8$

B: experimentally determined

- Btw. metal and non-metal
- <u>non-directional bond</u>
- High E (600 – 1500 KJ/mol)
- High T_m (melting)

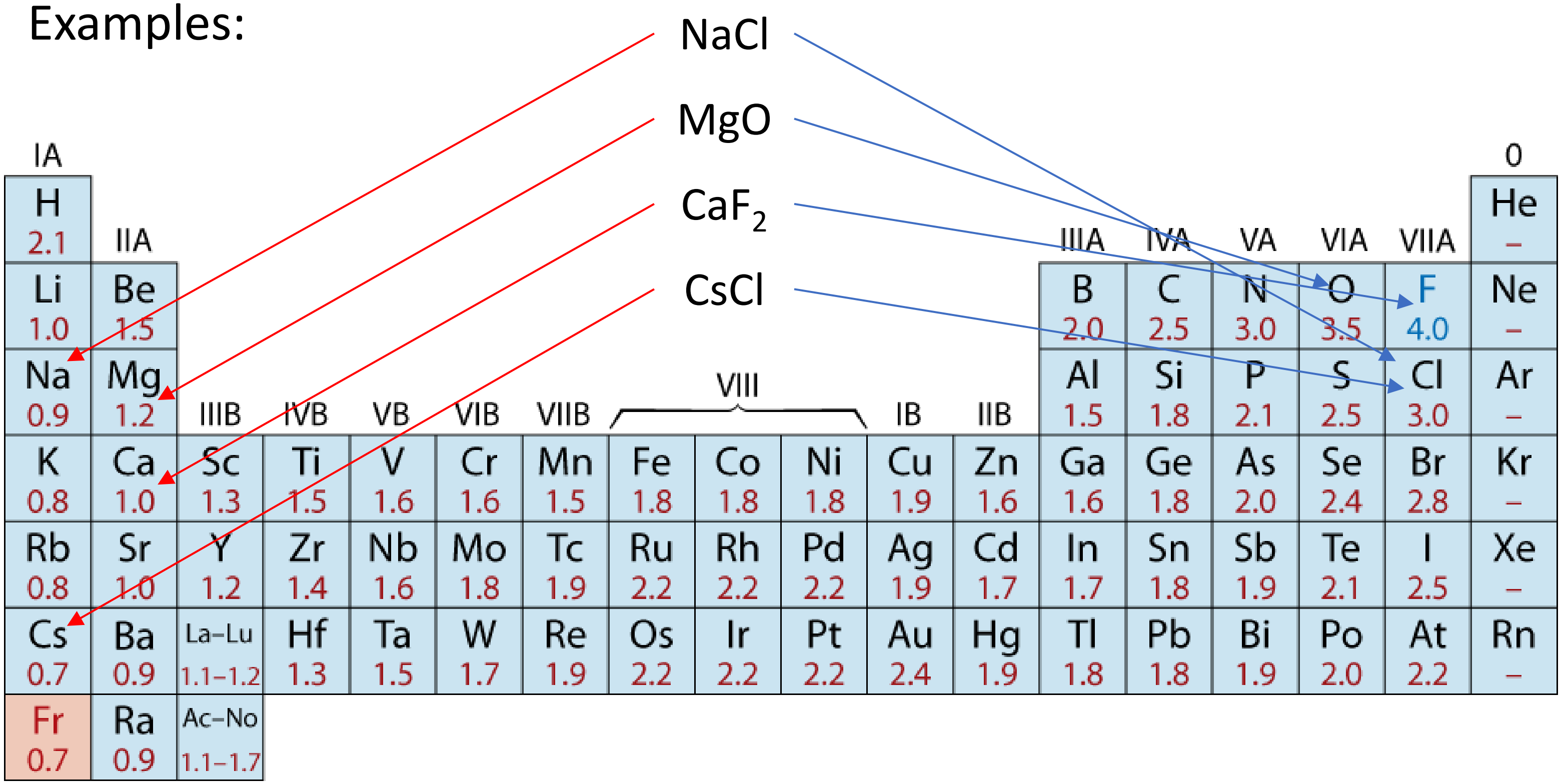


(b)

Ionic Bonding

Predominant bonding in Ceramics

Examples:



Smaller electronegativity

Larger electronegativity

IONIC BONDING

Predominant bonding in Ceramics

- hard and brittle
- electrically and thermally insulative

Bonding Energies and Melting Temperatures for Various Substances

Substance	Bonding Energy (kJ/mol)	Melting Temperature (°C)
	Ionic	
NaCl	640	801
LiF	850	848
MgO	1000	2800
CaF_2	1548	1418

Covalent Bonding

- Similar electronegativities share electrons
- Bonds involve valence electrons – normally *s* and *p* orbitals are involved
- directional bonding

Example: H_2

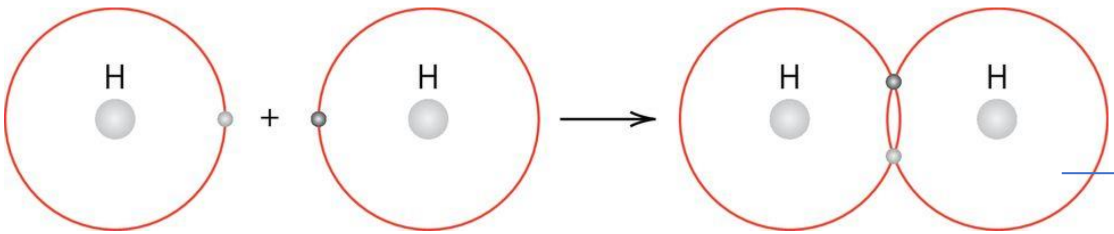


Fig. 2.12, *Callister & Rethwisch 10e.*

Proper phys. description
molecular orbitals

Molecules of non-metal elements: H_2, Cl_2, F_2

Heteroatomic molecules: HNO_3, CH_4, H_20,…

Solid elements: C (diamond), Si, Ge, Bi ….

Compounds: AsGa, InSb, SiC,…

Covalent Bonding

MATERIALS with COVALENT BONDING

Great variability!

C (diamond) T_m = 3550°C

AAAS Science

Bi T_m = 270°C

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Electrical properties:
insulators or semiconductors

Mech. Properties:
difficult prediction of typ properties!

Substance	Bonding Energy (kJ/mol)	Melting Temperature (°C)
	Ionic	
NaCl	640	801
LiF	850	848
MgO	1000	2800
CaF_2	1548	1418
	Covalent	
Cl_2	121	−102
Si	450	1410
InSb	523	942
C (diamond)	713	>3550
SiC	1230	2830
	Metallic	
Hg	62	−39
Al	330	660
Ag	285	962
W	850	3414
	van der Waals[a]	
Ar	7.7	−189 (@ 69 kPa)
Kr	11.7	−158 (@ 73.2 kPa)
CH_4	18	−182
Cl_2	31	−101
	Hydrogen[a]	
HF	29	−83
NH_3	35	−78
H_2O	51	0

COVALENT BONDING: BOND HYBRIDIZATION IN CARBON

electronic configuration C: $1s^2 2s^2 2p^2$

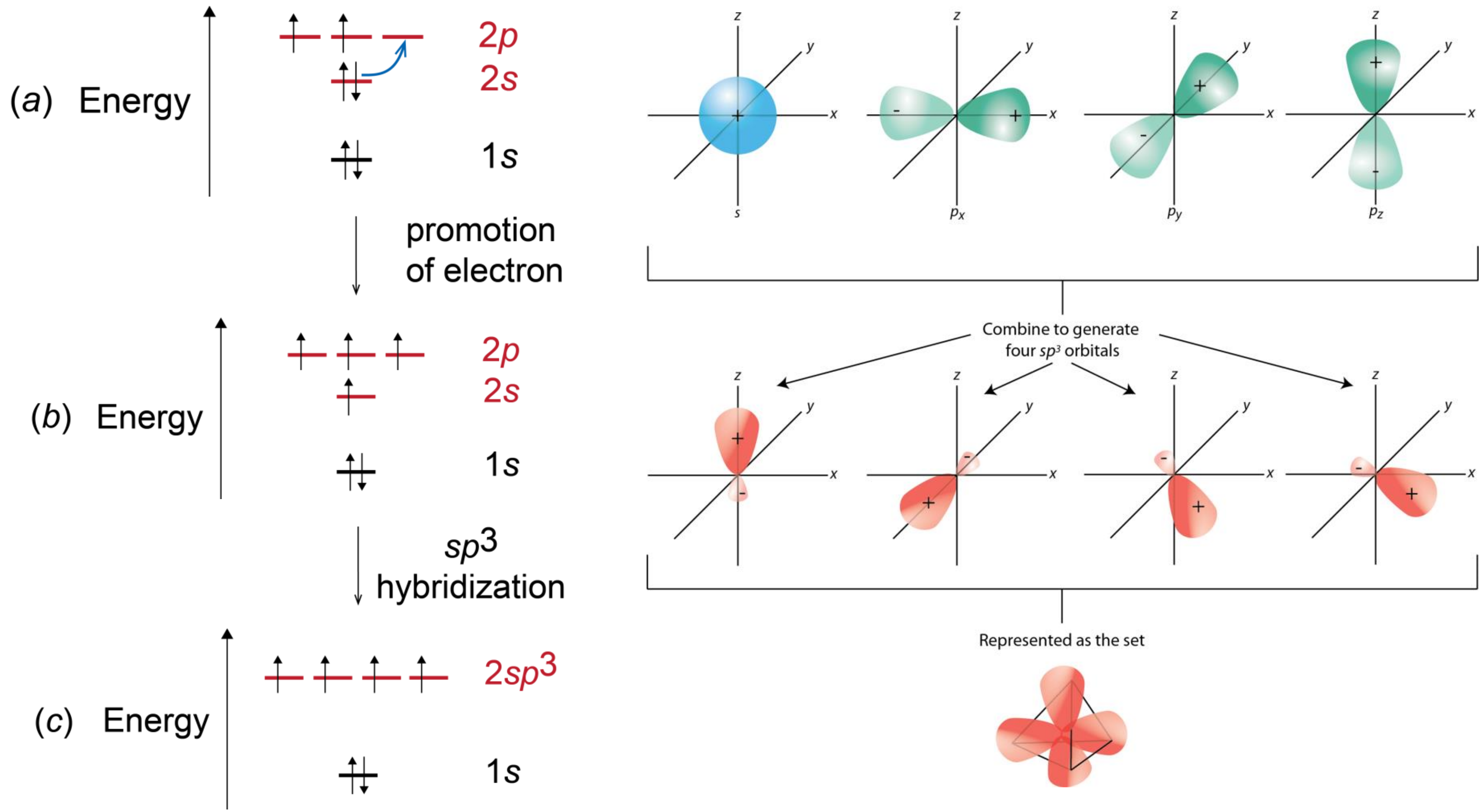


Fig. 2.13, *Callister & Rethwisch 10e.*

COVALENT BONDING: BOND HYBRIDIZATION IN CARBON

electronic configuration C: $1s^2 2s^2 2p^2$

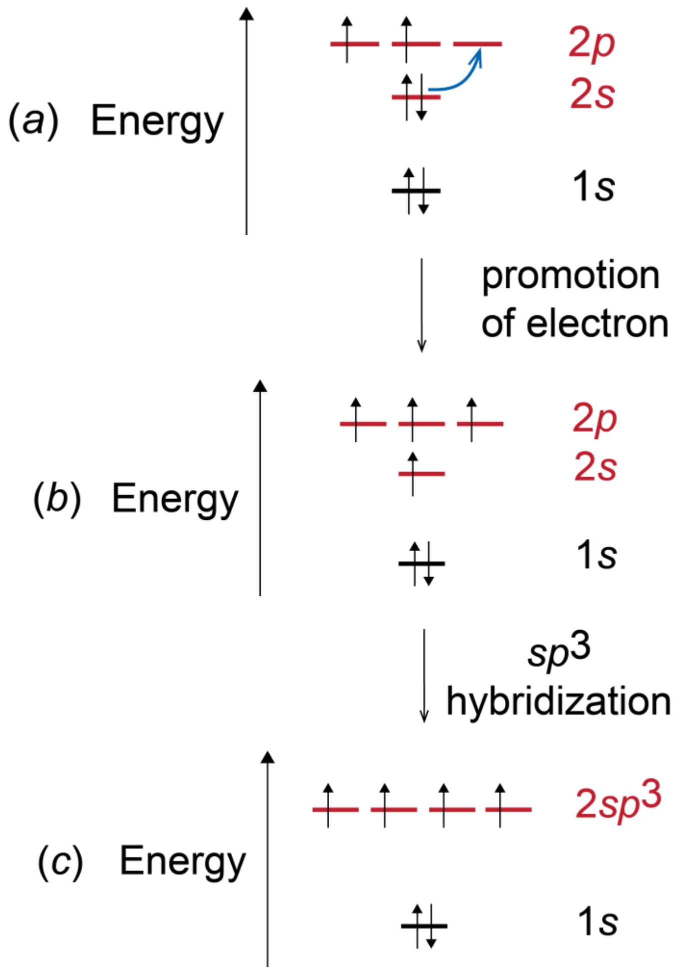


Fig. 2.13, *Callister & Rethwisch 10e.*

Carbon can form

<u>4 degenerate *sp*^{3} hybrid orbitals</u>

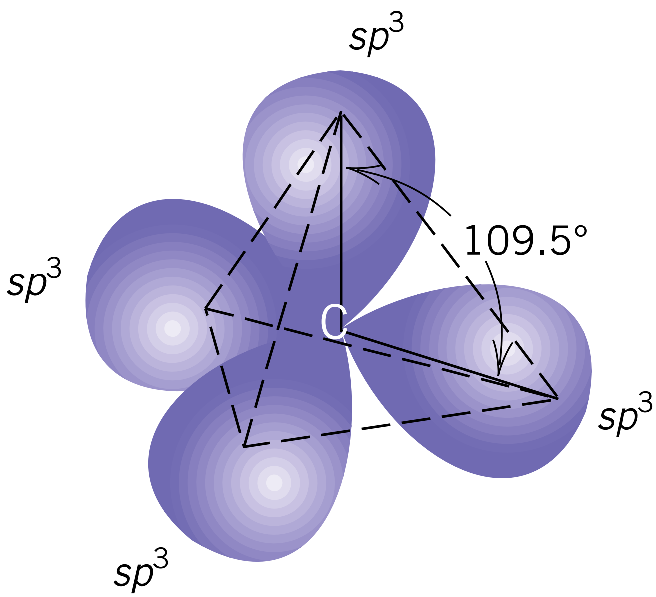


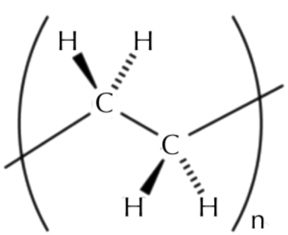
Fig. 2.14, *Callister & Rethwisch 10e.*
(Adapted from J.E. Brady and F. Senese, *Chemistry: Matter and Its Changes*, 4th edition. Reprinted with permission of John Wiley and Sons, Inc.)

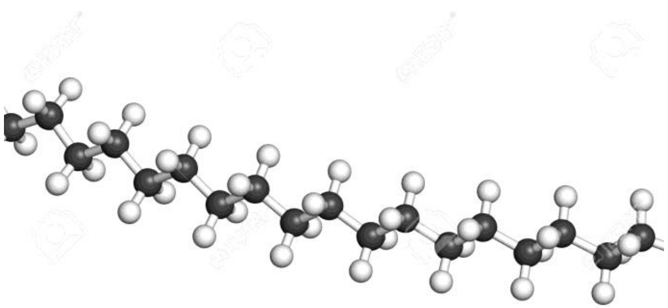
sp^3 HYBRIDIZATION IN CARBON

Hybrid *sp*^{3} bonding involving carbon

Electronegativities of C and H are similar so electrons are shared in *sp*^{3} hybrid covalent bonds.

- angle btw adjacent bonds: 109.5°
- zig-zag main chain in polymers!





Example: CH_4

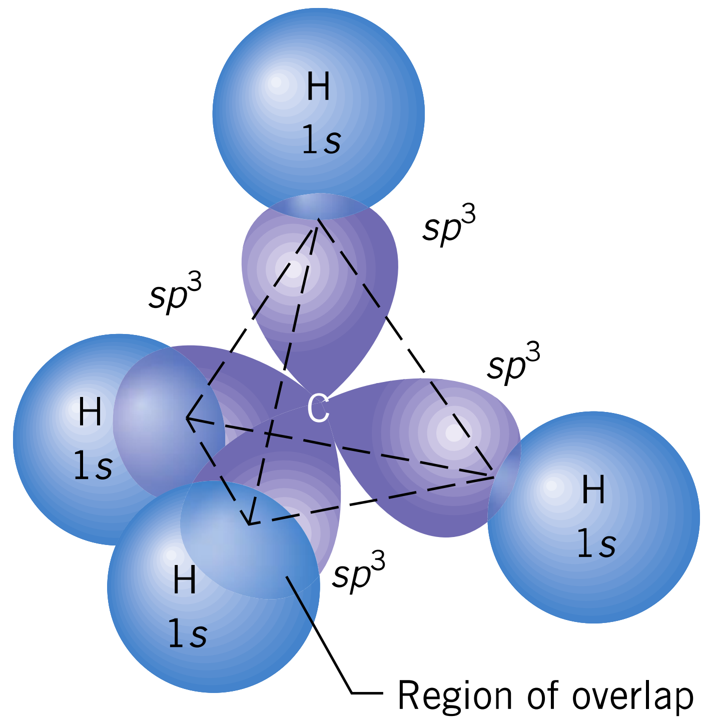


Fig. 2.15, *Callister & Rethwisch 10e.*
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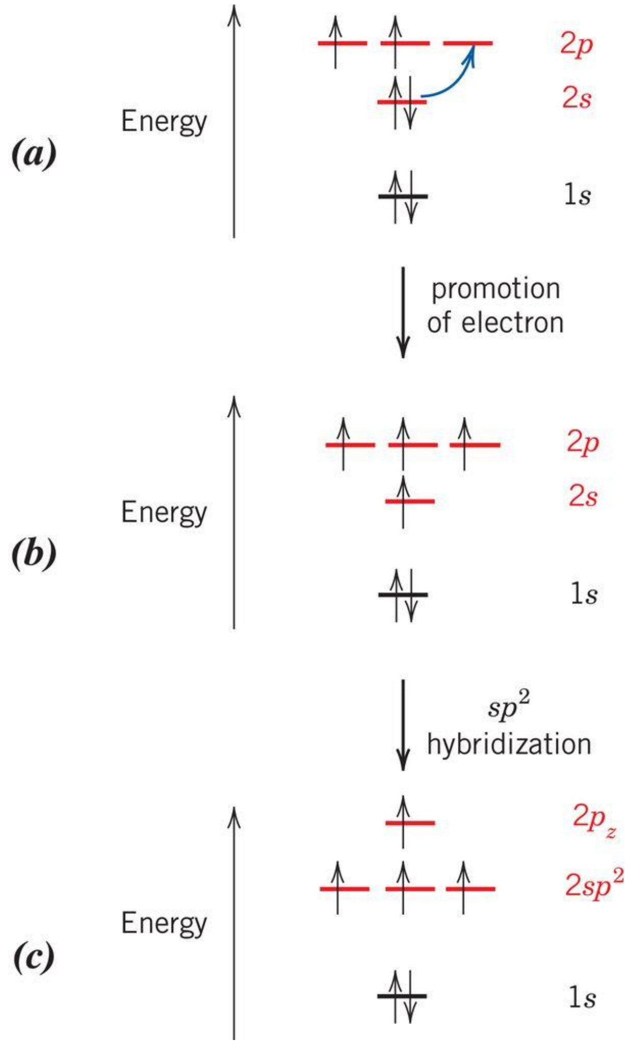
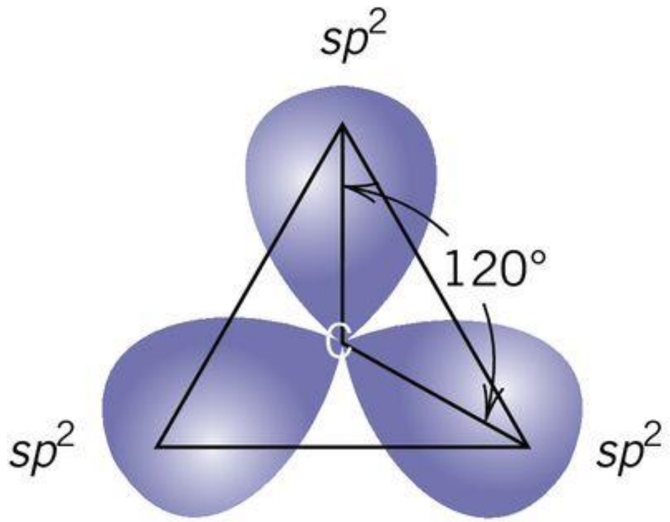
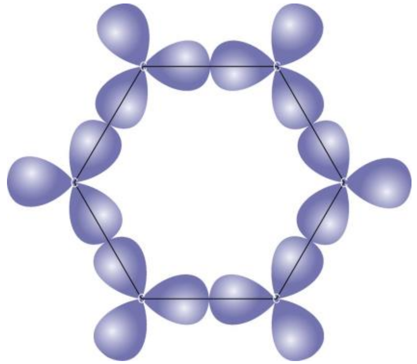
sp^2 HYBRIDIZATION IN CARBON



<u>3 degenerate sp^2 hybrid orbitals (in plane)</u>

1 pz orbital (out of plane)

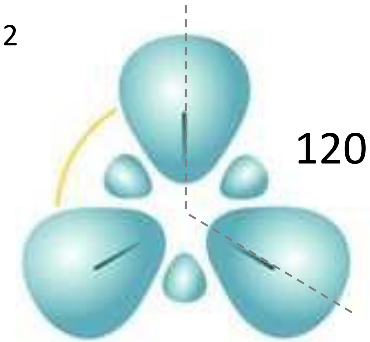




From J. E. Brady and F. Senese, *Chemistry: Matter and Its Changes*, 4th edition, 2004. Reprinted with permission of John Wiley & Sons, Inc.

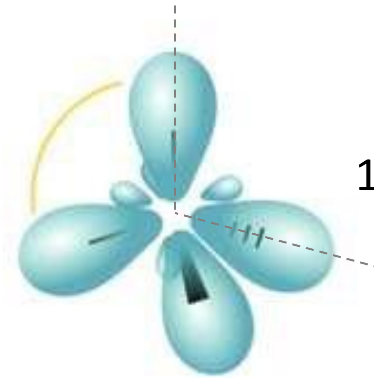
HYBRIDIZATION AND CARBON ALLOTROPES

sp^2



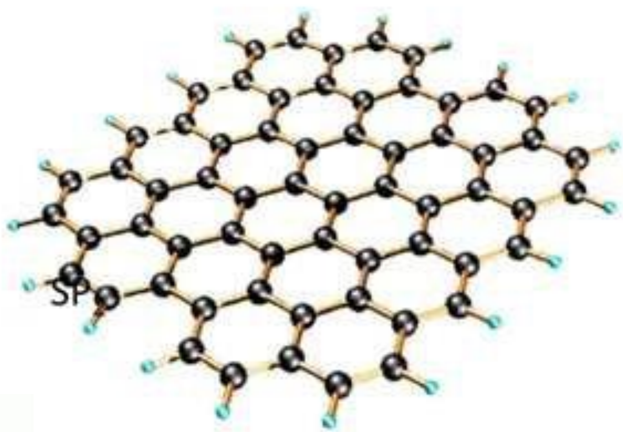
120°

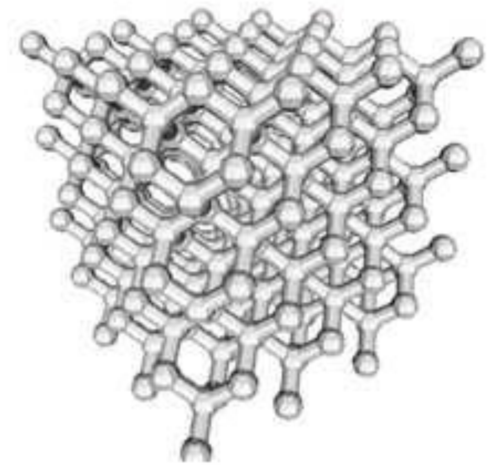
sp^3



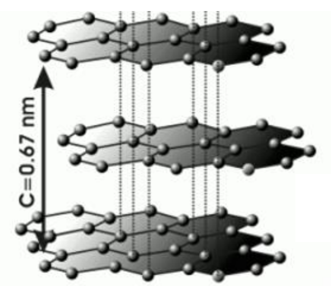
109.5°

trigonal planar



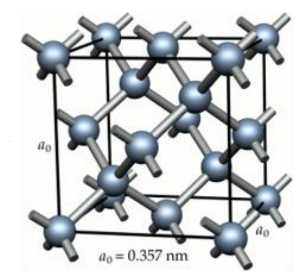


tetrahedral



Graphene, Graphite

Diamond



Bonding Energies and Melting Temperatures for Various Substances

Substance	Bonding Energy (kJ/mol)	Melting Temperature (°C)
	Ionic	
NaCl	640	801
LiF	850	848
MgO	1000	2800
CaF_2	1548	1418
	Covalent	
Cl_2	121	−102
Si	450	1410
InSb	523	942
C (diamond)	713	>3550
SiC	1230	2830

METALLIC BONDING

Electrons delocalized to form an "electron cloud"

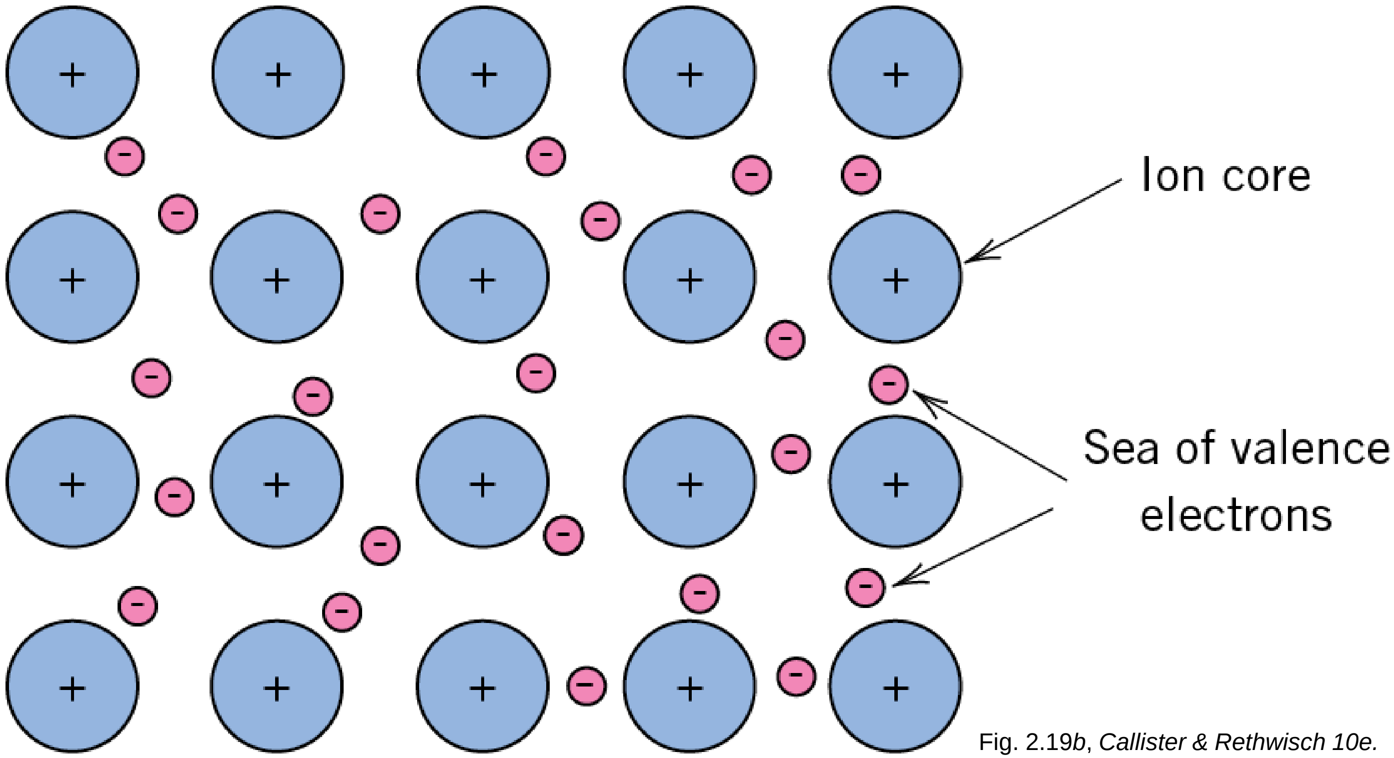


Fig. 2.19*b*, *Callister & Rethwisch 10e.*

Complete picture: **electron levels in a periodic potential** → BAND structure

as studied in Physics subjects: Structure of Matter, Solid State Physics

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METALLIC BONDING

- non-directional bonding
- Typ in groups IA, IIA, metals
- as a consequence of free electrons, metals are good electrical and thermal conductors
- ductile rupture at rt (=rupture after large permanent deformation)
- E_0, T_m not so high as in ionic
- Exceptions, e.g. W

Substance	Bonding Energy (kJ/mol)	Melting Temperature (°C)
	Ionic	
NaCl	640	801
LiF	850	848
MgO	1000	2800
CaF_2	1548	1418
	Covalent	
Cl_2	121	−102
Si	450	1410
InSb	523	942
C (diamond)	713	>3550
SiC	1230	2830
	Metallic	
Hg	62	−39
Al	330	660
Ag	285	962
W	850	3414
	van der Waals[a]	
Ar	7.7	−189 (@ 69 kPa)
Kr	11.7	−158 (@ 73.2 kPa)
CH_4	18	−182
Cl_2	31	−101
	Hydrogen[a]	
HF	29	−83
NH_3	35	−78
H_2O	51	0

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Cl_2	121	−102
Si	450	1410
InSb	523	942
C (diamond)	713	>3550
SiC	1230	2830
	Metallic	
Hg	62	−39
Al	330	660
Ag	285	962

L2.1.2

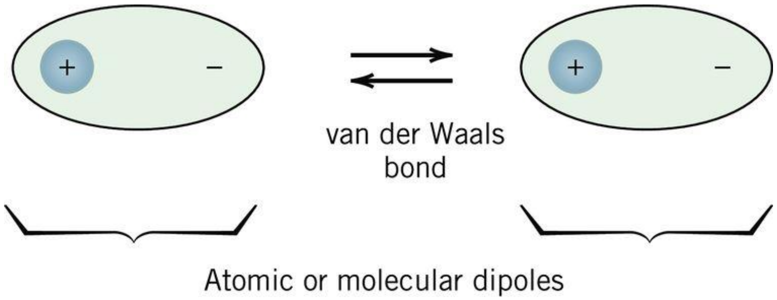
SECONDARY BONDS

SECONDARY BONDING - VDW

- extremely **weaker** than primary
- typ. 4-30 KJ/mol
- always present btw. atoms, molecules! but sometimes negligible in presence of primary bonding
- intermolecular

van der Waals forces

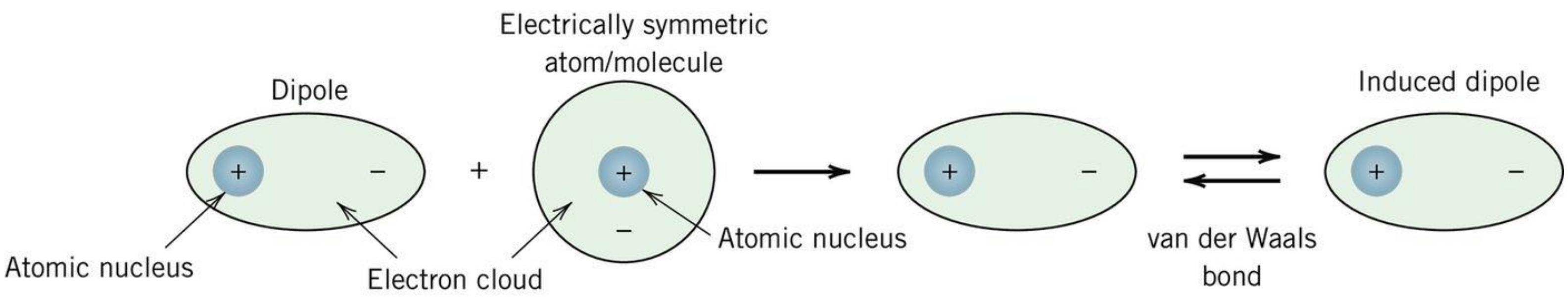
due to **dipolar interactions** between atoms, molecules



3 cases

Secondary Bonding - VdW

1. Fluctuating Induced Dipole Bonds (Dispersion Forces)



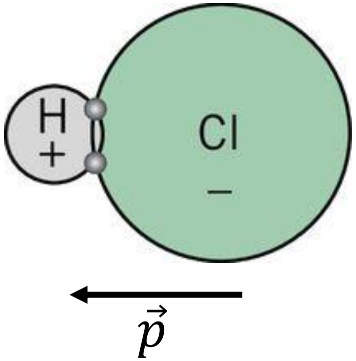
attractive forces, which are temporary and fluctuate with time, may exist between large numbers of atoms or molecules

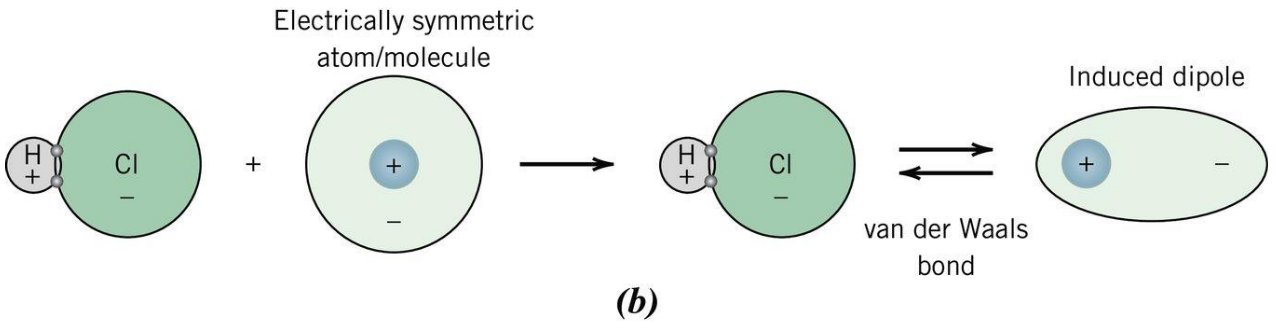
- liquefaction of inert gases and other electrically neutral and symmetric molecules (H_2 , Cl_2 , …)
- extremely low melting and boiling temperatures
- of all possible intermolecular bonds, these are the weakest

SECONDARY BONDING - VDW

2. Polar Molecule–Induced Dipole Bonds

polar molecule: a molecule having a pemanent dipole moment, due to asymettric arrangement of positive and negative charges



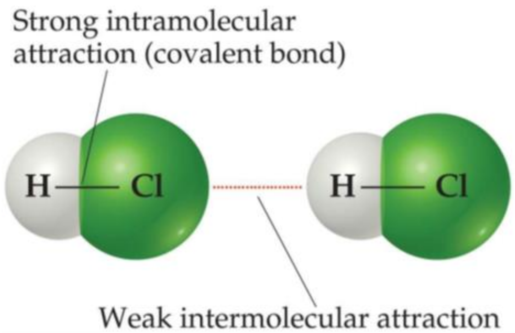


- bonding E larger than for fluctuating induced dipole

SECONDARY BONDING - VDW

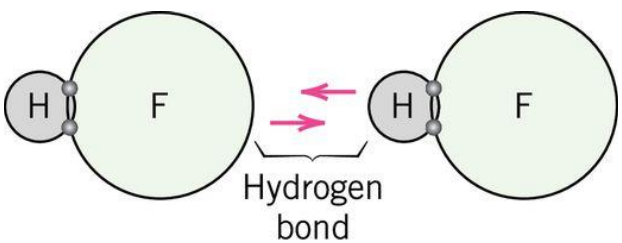
3. Permanent Dipole Bonds

- bonding E significantly greater than induced dipoles



www.unf.edu

SPECIAL CASE: **Hydrogen BONDING**



H-F
H-O
H-N

- strongest secondary bonding (E up to 51 KJ/mol)

VdW forces in action!

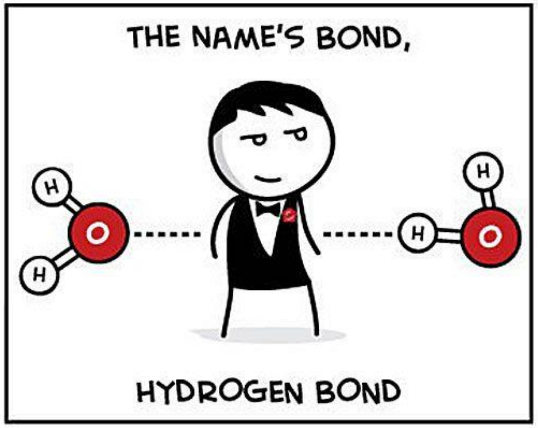
(08:54)

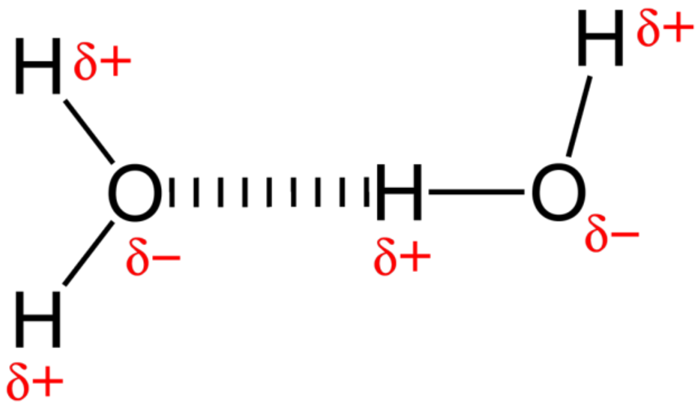
YOUTUBE VIDEO - Be Smart Channel
«The Lizard That Uses Nanotechnology to Walk Upside Down”

https://youtu.be/p6QmV1EbVnI

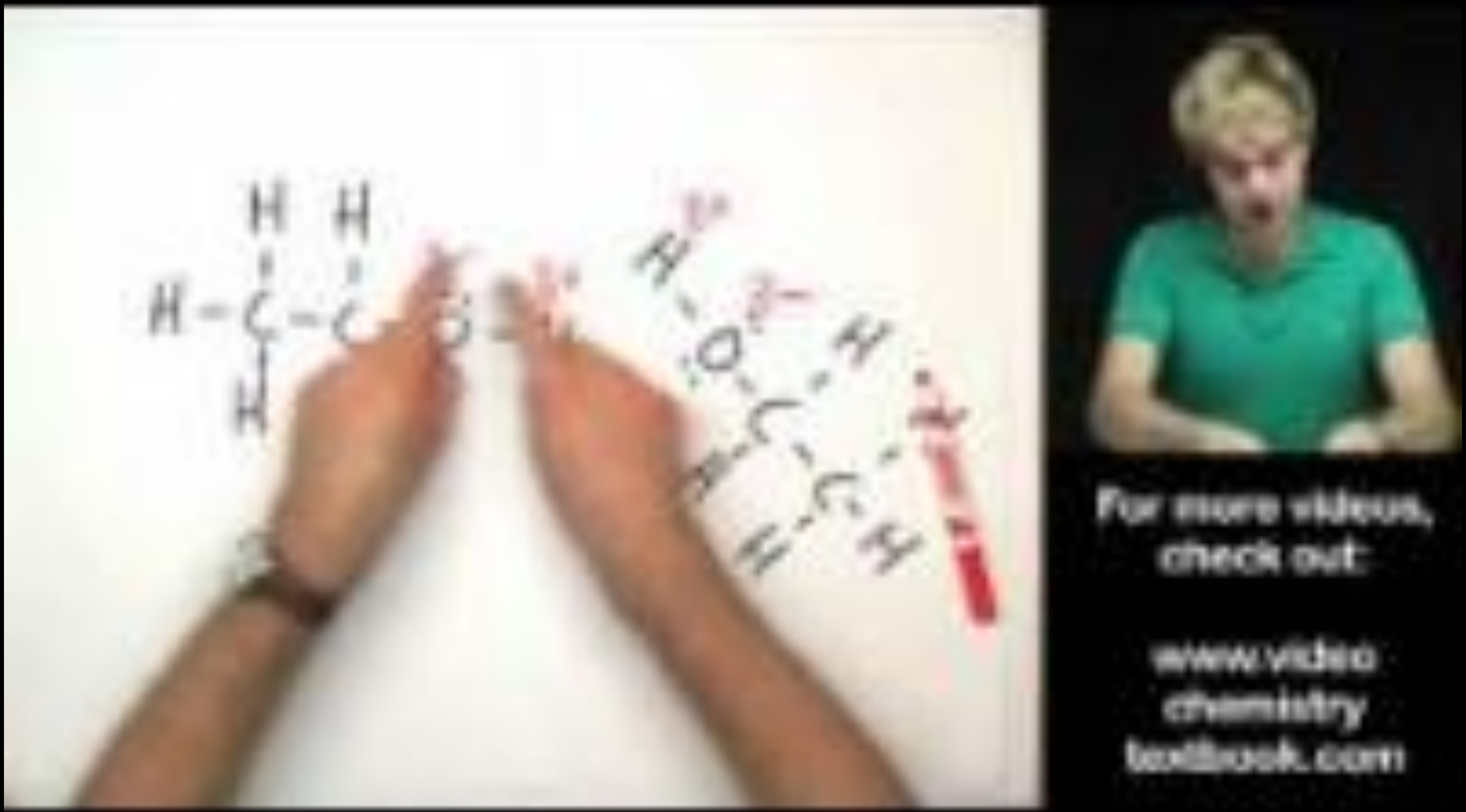
HYDROGEN BONDING: WATER

- extremely important for water properties!
- biomaterials





Hydrogen Bonding

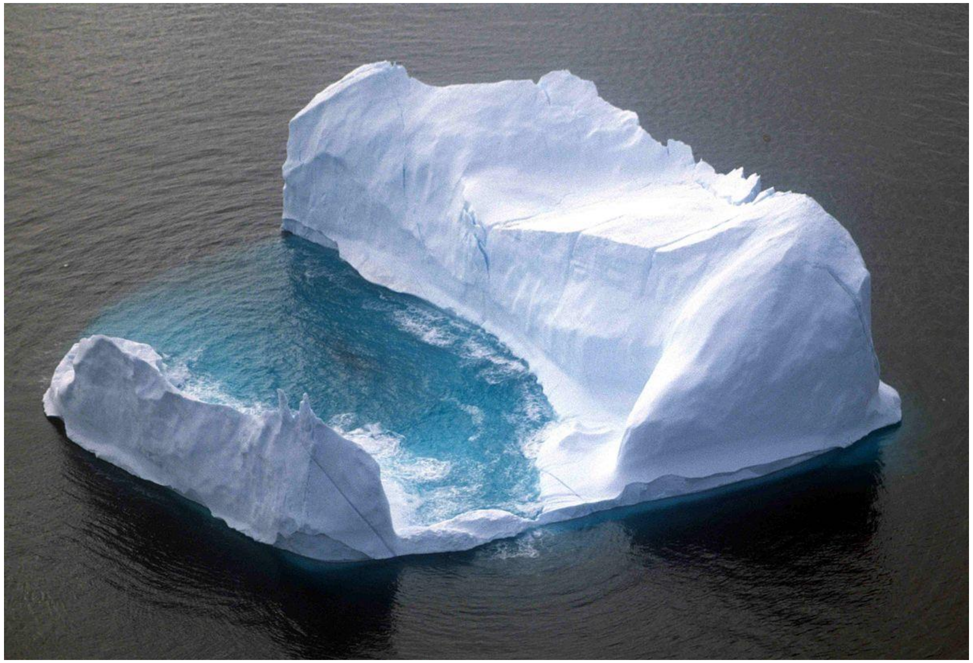


YOUTUBE VIDEO (09:00)

Hydrogen bonding and common mistakes

https://youtu.be/PyC5r2mB4d4

QUESTION



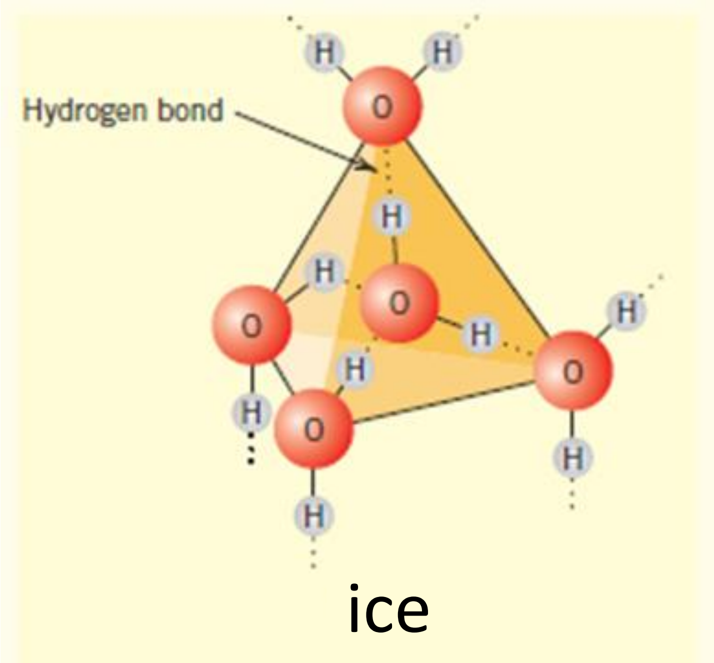
Why do icebergs float?

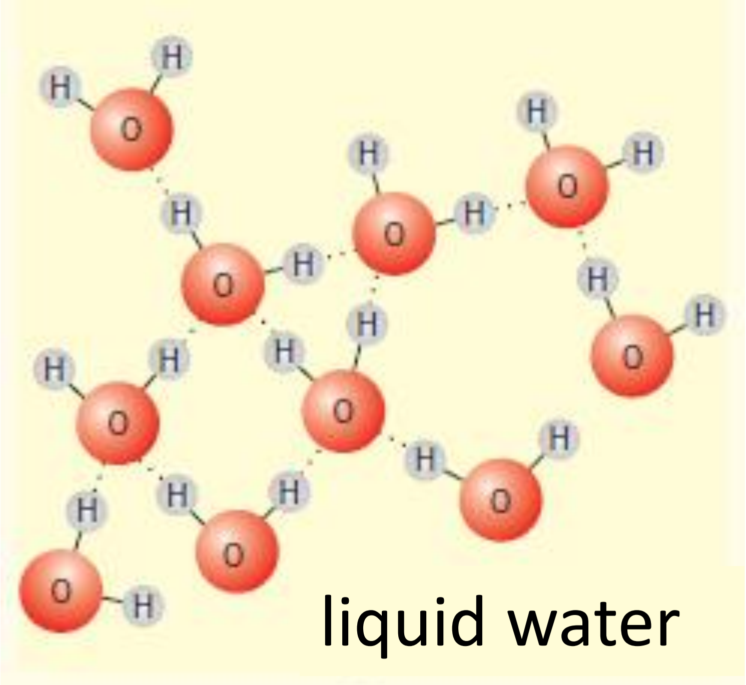
WHY DOES ICE FLOAT IN WATER?

TEDEd VIDEO (Animation) (available on YOUTUBE too)
Why Does Ice float in water? (03:55)

https://youtu.be/UukRgqzk-KE

WATER DENSITY AND CN





CN: 4

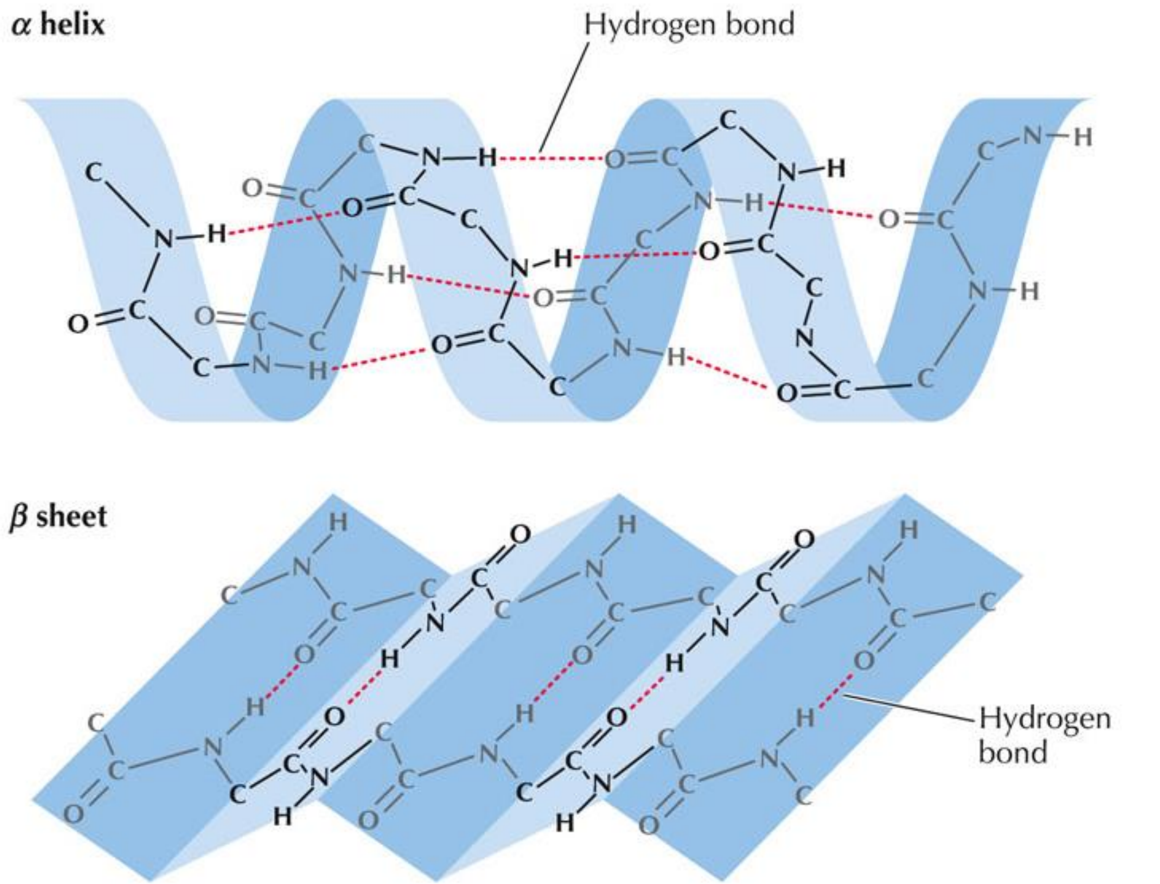
d=0.917 g/ml

CN: 4.5

d=1.0 g/ml

Hydrogen bonding: Polymers

Polypeptides (Proteins)

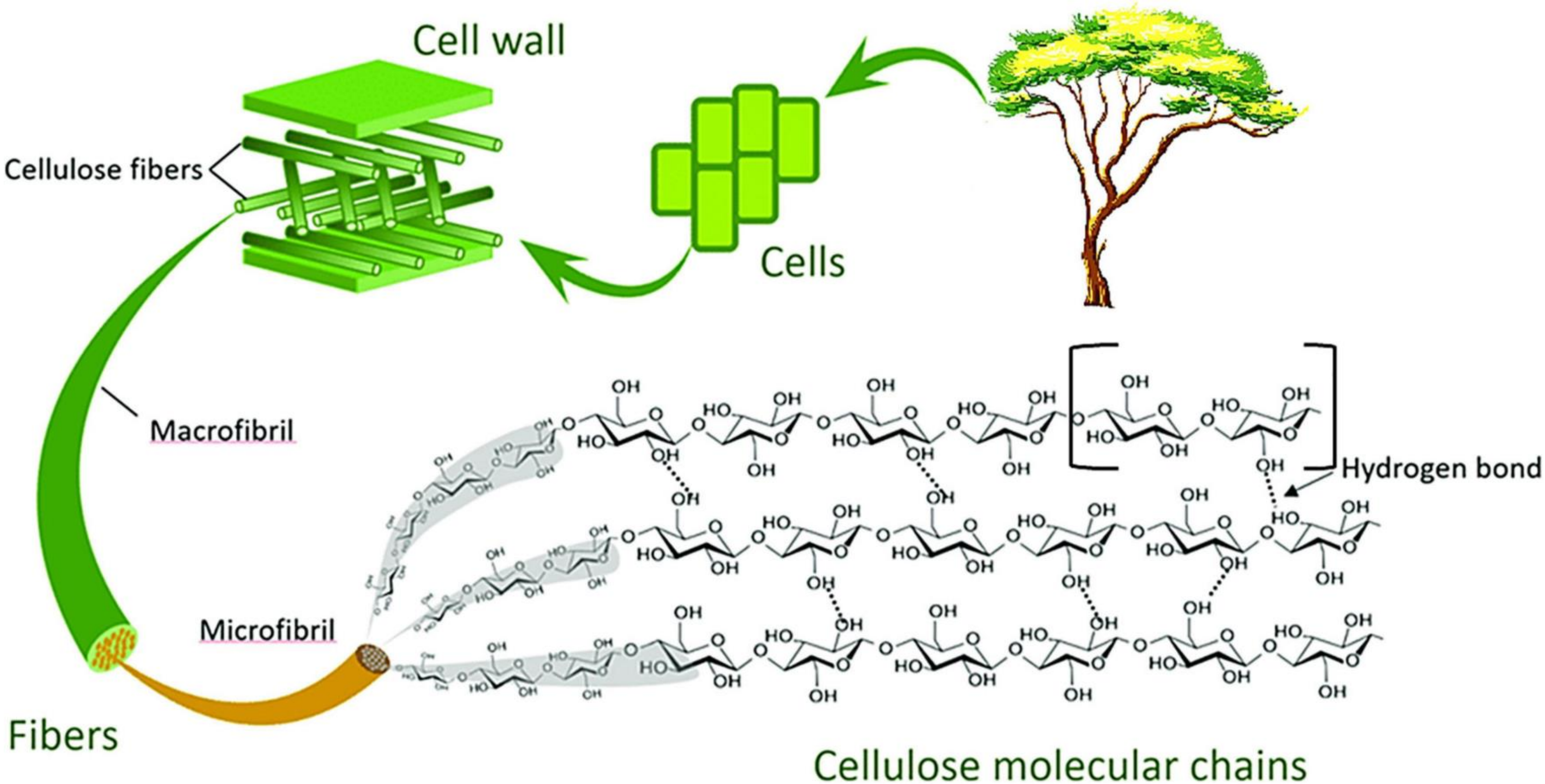


THE CELL, Fourth Edition, Figure 2.19 © 2006 ASM Press and Sinauer Associates, Inc.

Hydrogen Bonding: Polymers

Polysaccharides: Cellulose

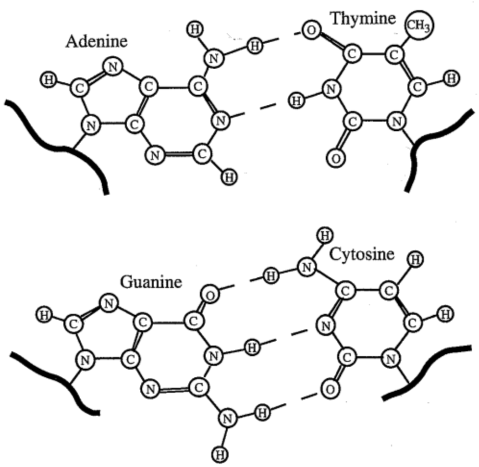
- polymer-polymer interaction
- polymer-water interaction

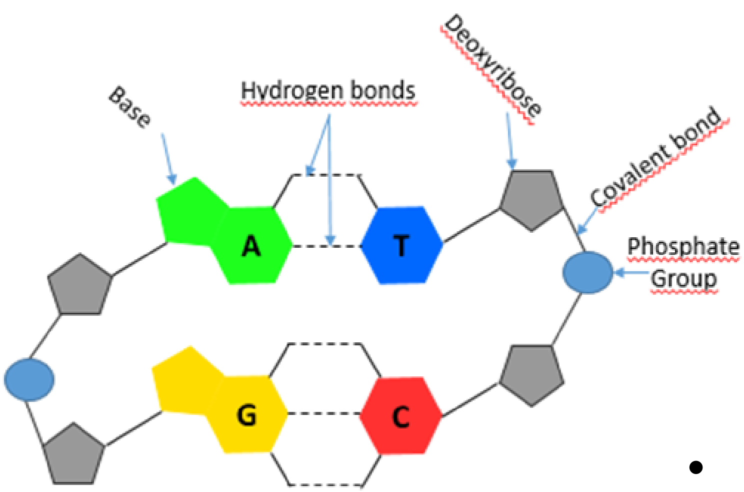


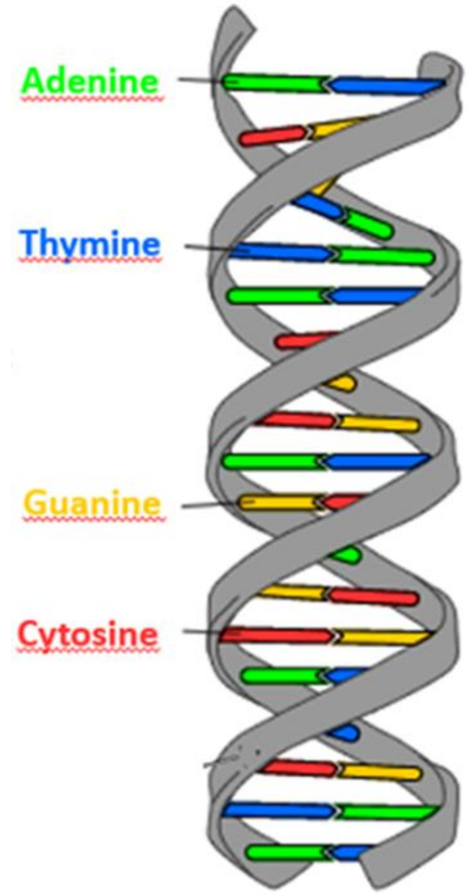
Frontiers En. Res. 2021 https://doi.org/10.3389/fenrg.2021.608825

Hydrogen Bonding: Polymers

DNA







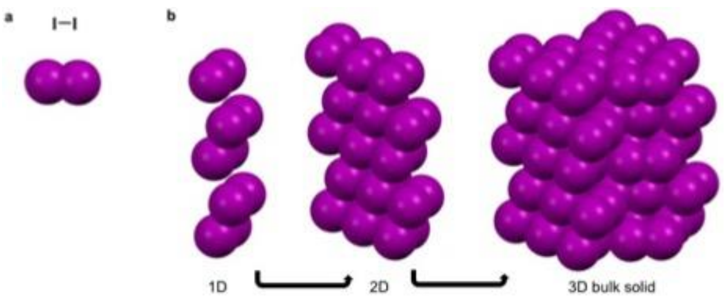
- DNA strands (double helix) are held together by H-bond btw. bases

Substance	Bonding Energy (kJ/mol)	Melting Temperature (°C)
	van der Waals[a]	
Ar	7.7	−189 (@ 69 kPa)
Kr	11.7	−158 (@ 73.2 kPa)
CH_4	18	−182
Cl_2	31	−101
	Hydrogen[a]	
HF	29	−83
NH_3	35	−78
H_2O	51	0

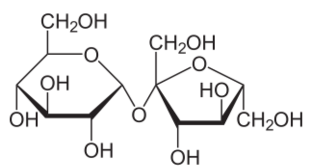
MOLECULES: CONDENSED STATES

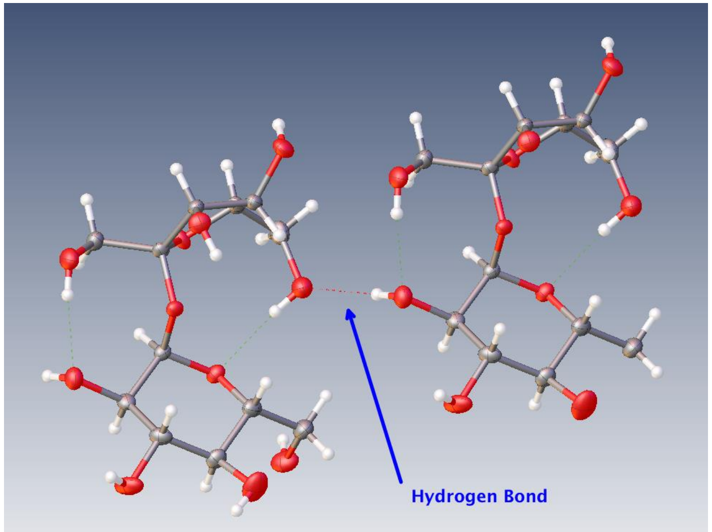
- liquid and solid state of molecules:
  - elemental diatomic molecules (F_2, O_2, H_2, I_2 etc.)
  - compounds (H_2O, CO_2, HNO_3, C_6H_6, CH_4, etc.)
- bonds between molecules are weak secondary ones
  - van der Waals forces
  - dipole-dipole interactions
  - quadrupole interactions
  - π-π interactions
  - hydrogen bonding/halogen bonding
  - London dispersion forces

Ex: solid I_2 (dispersion forces)



Ex:
Sucrose





physicsstackexchange.org

Molecular Solids

- small molecules: soft, often volatile, low T_m,

  electrical insulators

- larger molecules: less volatile, higher T_m

- extreme: modern polymers

dispersion forces increase with the larger number of atoms

Melting points of some molecular solids[41][42] hide

Formula	T_m °C
H_2	−259.1
F_2	−219.6
O_2	−218.8
N_2	−210.0
CH_4	−182.4
C_2H_6	−181.8
C_3H_8	−165.0
C_4H_{10}	−138.3
C_5H_{12}	−129.8
Cl_2	−101.6
C_6H_{14}	−95.3
HBr	−86.8
HF	−80.0
NH_3	−80.0
HI	−50.8
$C_{10}H_{22}$	−29.7
HCl	−27.3
Br_2	−7.2
H_2O	0.0
C_6H_6	5.5
I_2	113.7
S_8	119.0
C_6Cl_6	220.0

Mixed Bonding

Most common mixed bonding type is <u>Covalent-Ionic</u> mixed bonding

$$\% \text{ ionic character} = \left(1 - e^{-\frac{(X_A - X_B)^2}{4}}\right) \text{x } (100 \ \%)$$

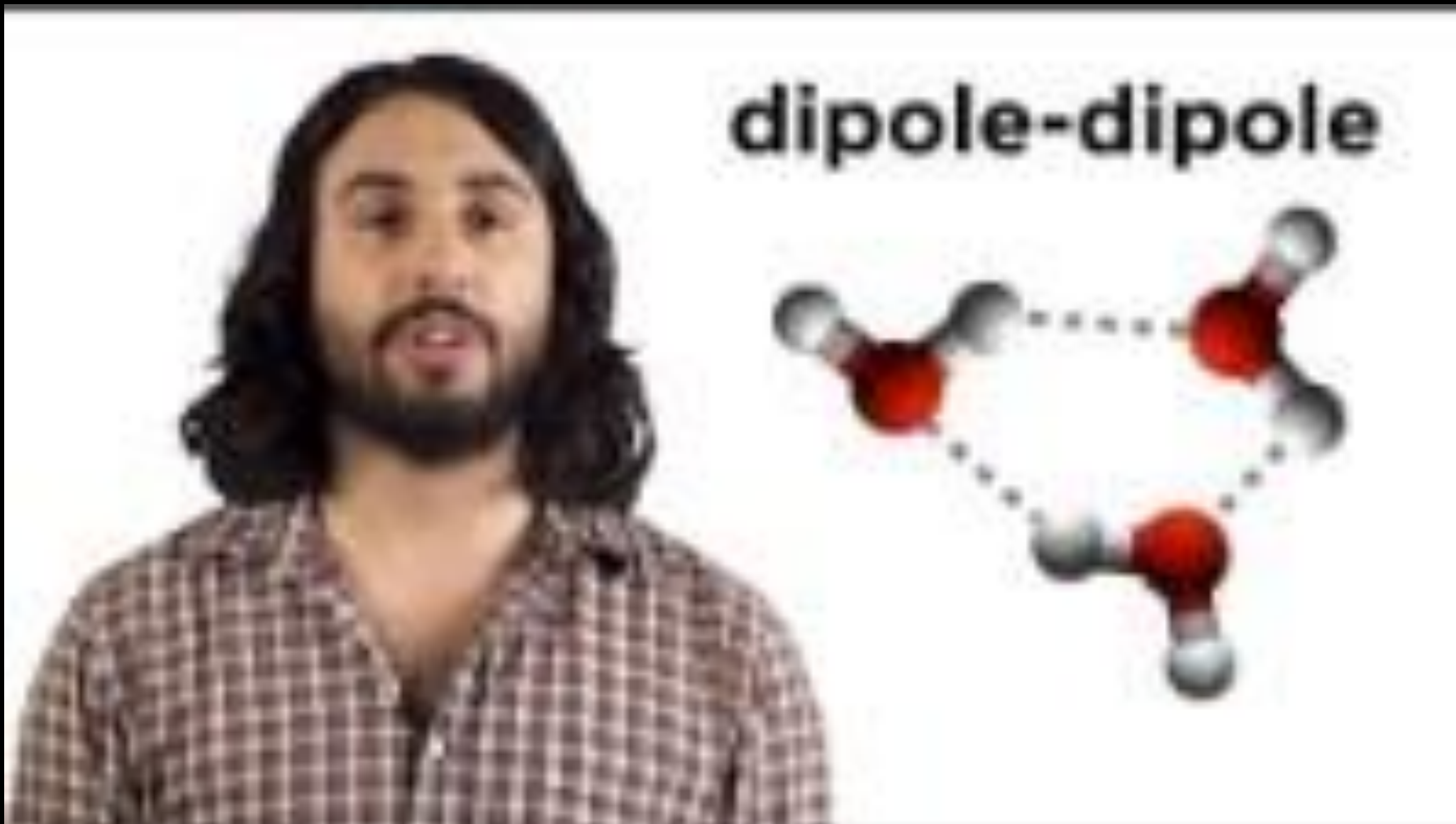
X_A , X_B : electronegativities of the two elements participating in the bond

Example: MgO $\quad X_{Mg} = 1.2$

$X_O = 3.5$

$$\% \text{ ionic character} = \left(1 - e^{-\frac{(3.5-1.2)^2}{4}}\right) \text{x } (100\%) = 73.3\%$$

A SIMPLE RECAP ON INTERMOLECULAR FORCES



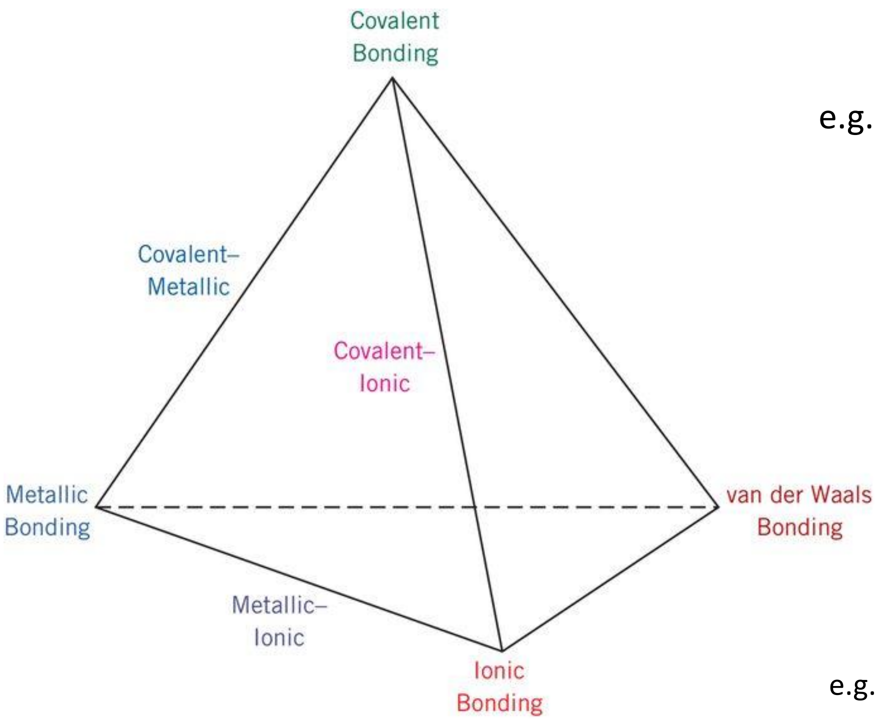
YOUTUBE VIDEO (10:55)
Channel «Professor Dave explains»
Intermolecular Forces and Boiling Points

https://youtu.be/08kGgrqaZXA

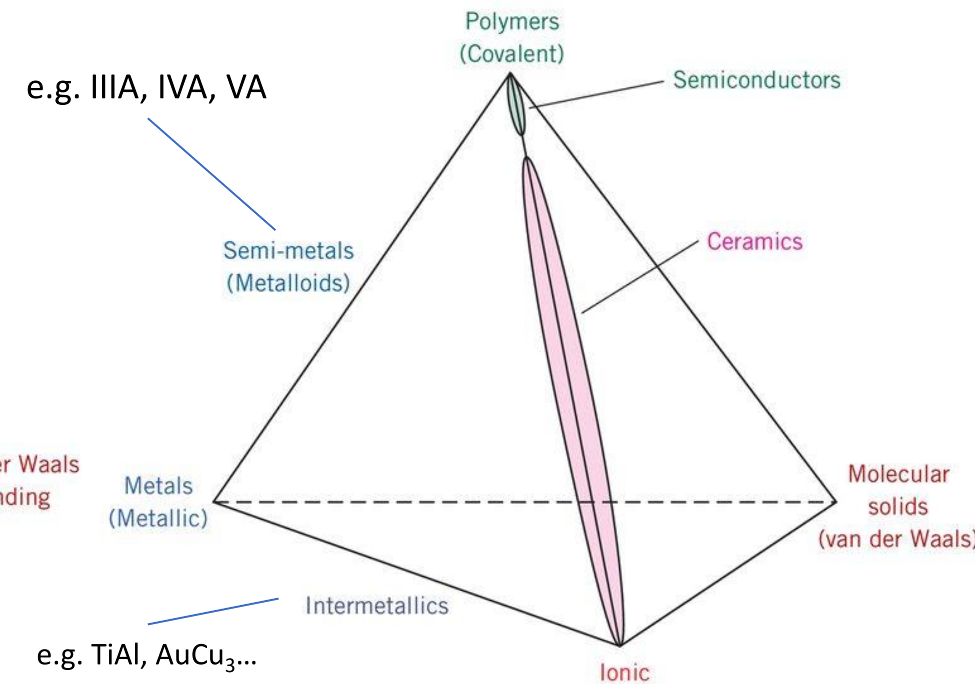
L2.1.3

Bonds and Materials Classes

Mixed Bonding – Materials Classes



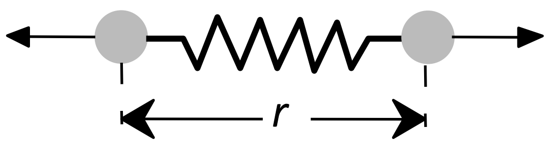
Bonding tetrahedron



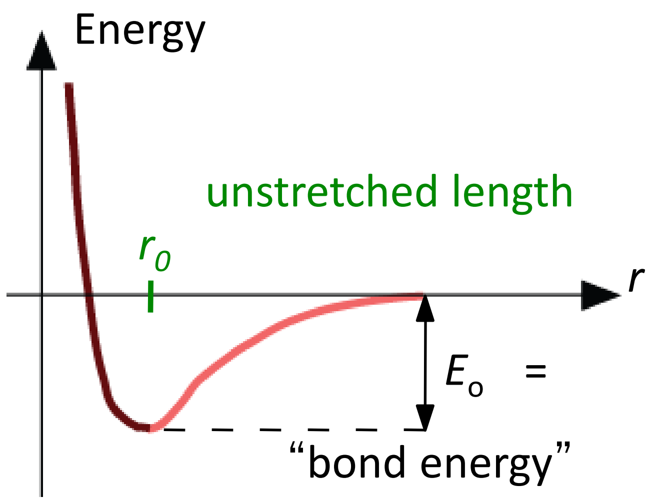
Materials-type tetrahedron

Properties Related to Bonding I: Melting Temperature (T_M)

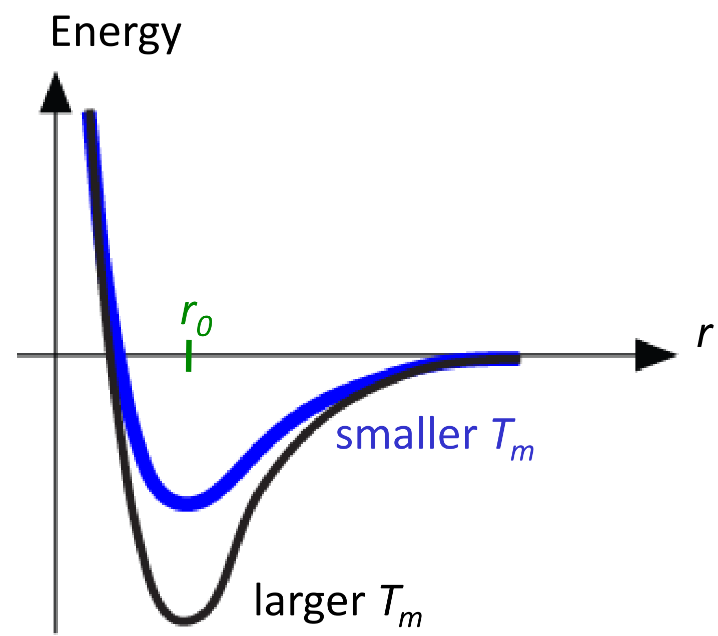
- Bond length, r



- Bond energy, E_o

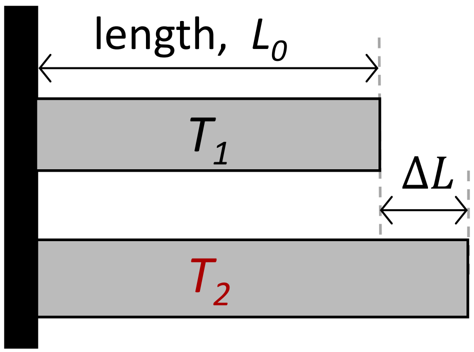


- Melting Temperature, T_m



The larger E_o, the higher T_m

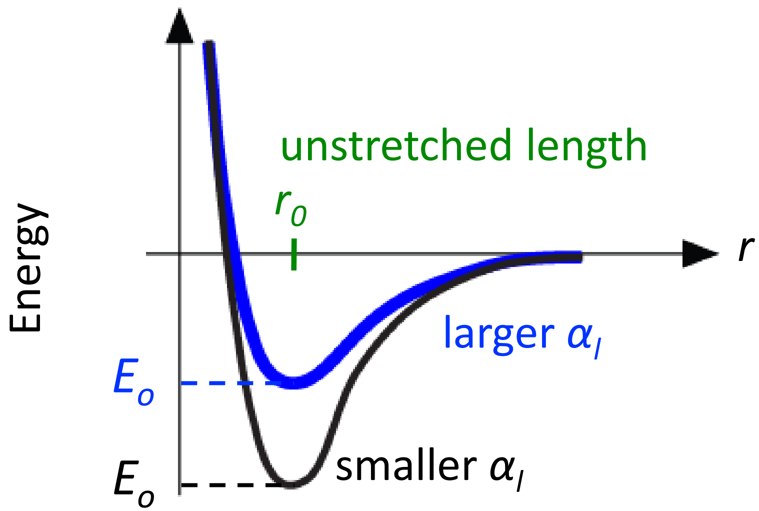
PROPERTIES RELATED TO BONDING II:
COEFF. OF THERMAL EXPANSION



$T_1 < T_2$

$$\frac{\Delta L}{L_0} = \alpha_l (T_2 - T_1)$$

The smaller E_o, the larger α_l

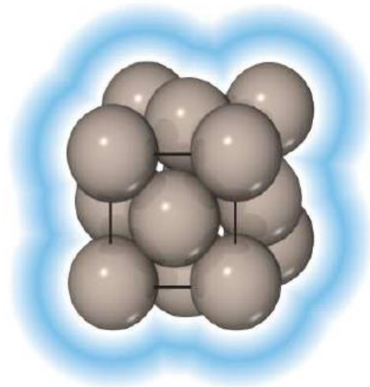


- increase in bond length due to asymmetry of the E (r) curve → incr. α_l
- as E_0 increases this asymmetry decreases

SOLIDS & PROPERTIES

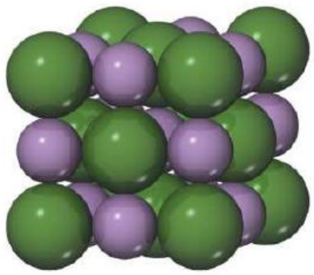
classifications of solids based on bonding

- var. T_m
- var. hardness
- conductors



Metallic solids

Extended networks of atoms held together by metallic bonding (Cu, Fe)

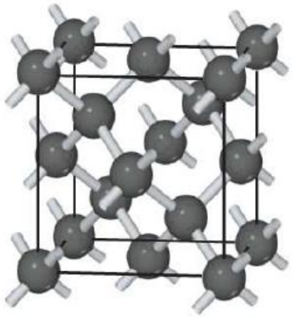


Ionic solids

Extended networks of ions held together by ion–ion interactions (NaCl, MgO)

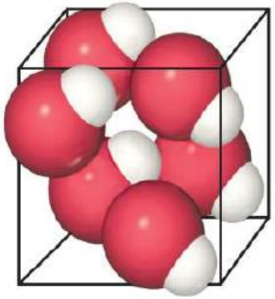
- high T_m
- hard, brittle
- insulators

- rel. high T_m
- hard
- insul/ semiconductors



Covalent-network solids

Extended networks of atoms held together by covalent bonds (C, Si)



Molecular solids

Discrete molecules held together by intermolecular forces (HBr, H_2O)

- low T_m
- insulators

SOLIDS & PROPERTIES

classifications of solids based on materials classes

Ceramics

(Ionic & covalent bonding):

Large bond energy
- high T_m
- large E
- small α_l

Metals

(Metallic bonding):

Variable bond energy
- moderate T_m
- moderate E
- moderate α_l

Polymers

(Covalent & Secondary):

Weak bond energy (between chains)
Secondary bonding responsible for most physical properties
- low T_m
- small E
- large α_l

SOLID OR LIQUID?

YOUTUBE video 1 https://youtu.be/2mYHGn_Pd5M?t=13

YOUTUBE video 2 https://youtu.be/BleCJJAKkgw?t=4

"Normal" condensed matter

SOLID LIQUID

More on this in next lectures

"Soft" condensed matter

?

....more difficult to classify

SUMMARY L2

- A material's chemical, electrical, thermal, and optical properties are determined by **electronic configuration** (valence electrons in outermost unfilled shells).
- **Primary bonding** types include: covalent, ionic, and metallic bonding.
- **Secondary or van der Waals bonds** are weaker than the primary bonding types.
- The percent ionic character of a **covalent-ionic mixed bond** between two elements depends on their electronegativities.
- Knowing the bonding in a solid we can have a rough estimate of its properties

ADDITIONAL RESOURCES, READINGS

VIDEO/INTERACTIVE RESOURCES:

- The Periodic Videos , by TEDEd – https://ed.ted.com/periodic-videos
  a video for each element of the periodic table!

- Youtube video «Hydrogen bonding and common mistakes - https://youtu.be/PyC5r2mB4d4

- just for fun…tons of funny/instructive videos on YouTube about «strange» fluids: non-newtonian fluids, magnetorheological, electrorheological fluids

READINGS:

- Callister Rethwisch – Chapter 2

ADDITIONAL RESOURCES

- for going much more in depth (not necessary for the exam!)

Molecular Solid - WIKIPEDIA

Madelung Constant (Ionic solids) - WIKIPEDIA

Bulk modulus (microscopic origin)- WIKIPEDIA

COHESIVE ENERGY IN SOLIDS

SLIDES from Course «Solid State Physics», Prof. Peter Hadley, TUGraz

Institute of Solid State Physics KI

3.1.3 From the interatomic potential (pair of atoms) to the cohesive energy (the crystal)

Cohesive energy (neglecting kinetic energy of the noble gas atoms):

$$U_{tot} = \frac{1}{2} N 4\varepsilon \left\{ \sum_j{}' \left(\frac{\sigma}{p_{ij} R} \right)^{12} - \sum_j{}' \left(\frac{\sigma}{p_{ij} R} \right)^{6} \right\}$$

Independent of the chosen "i"!

with: $r_{ij} = p_{ij} R$

add energetic contributions of all atoms, but avoid double counting

summation over all "other" atoms

distance between reference atom i and all other atoms (R ... nearest-neighbor distance)

Evaluate for fcc structure: $\sum_j{}' \frac{1}{p_{ij}^{12}} = 12.1318$ $\quad \sum_j{}' \frac{1}{p_{ij}^{6}} = 14.4539$

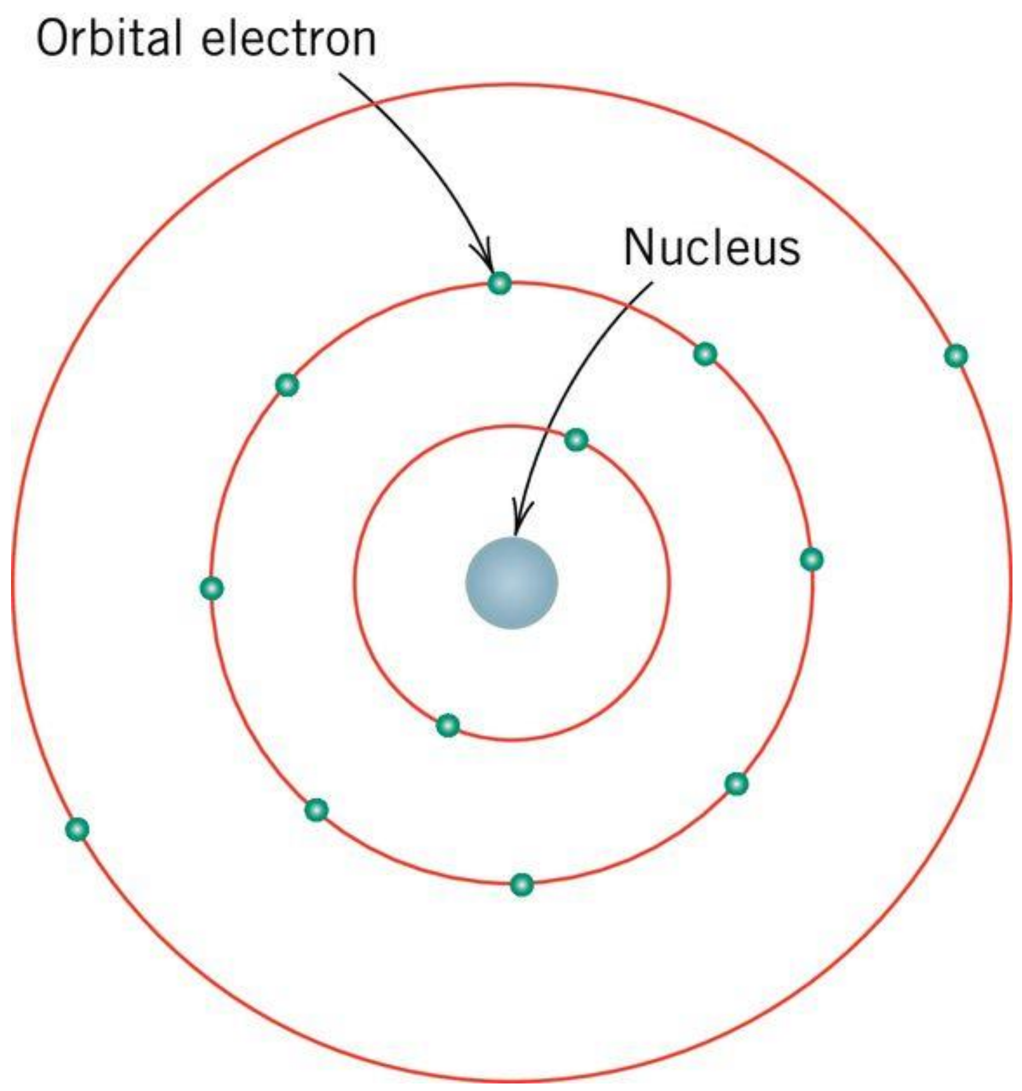
Close to number of nearest neighbors in fcc structure (i.e., 12)

→ the nearest neighbours count primarily !

Fundamentals of Solid State Physics

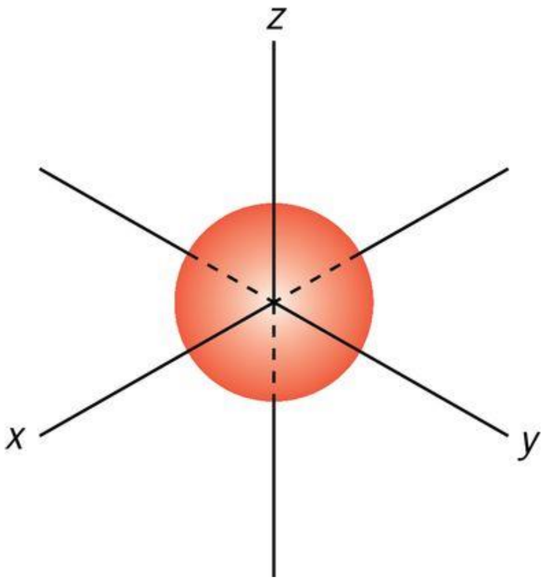
RESERVE SLIDES

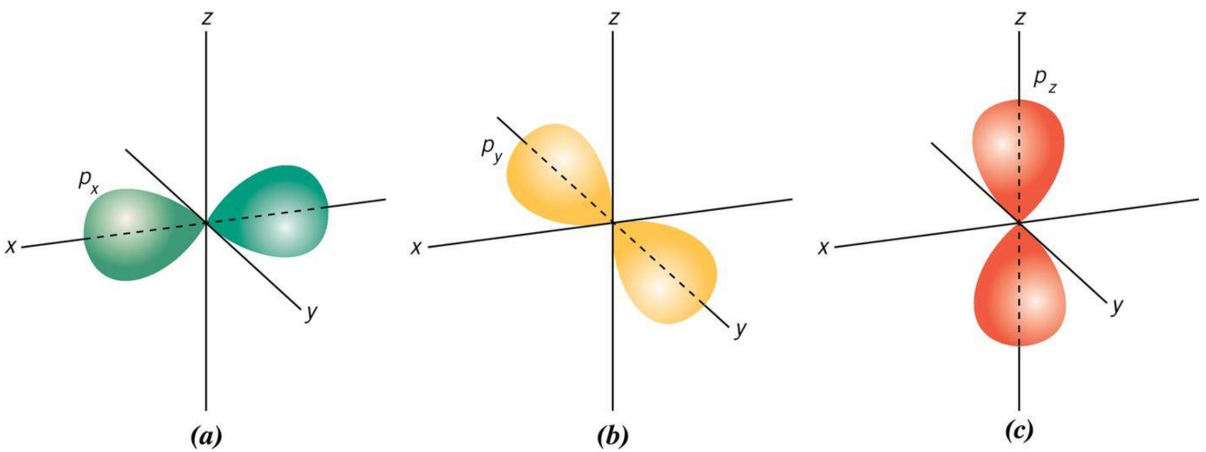
- Atoms, orbitals


Orbital electron
Nucleus

s orbital

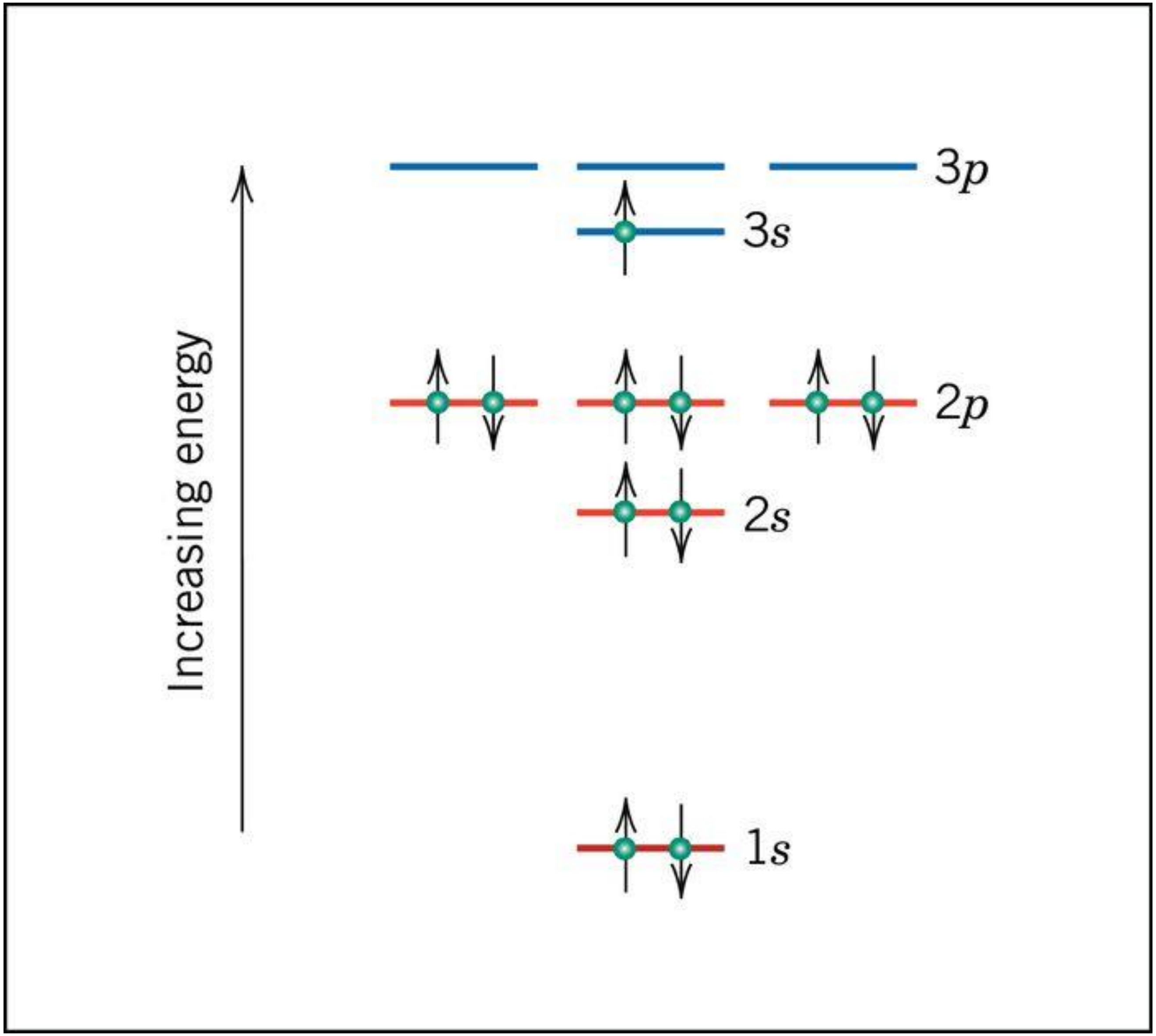
3 p orbitals

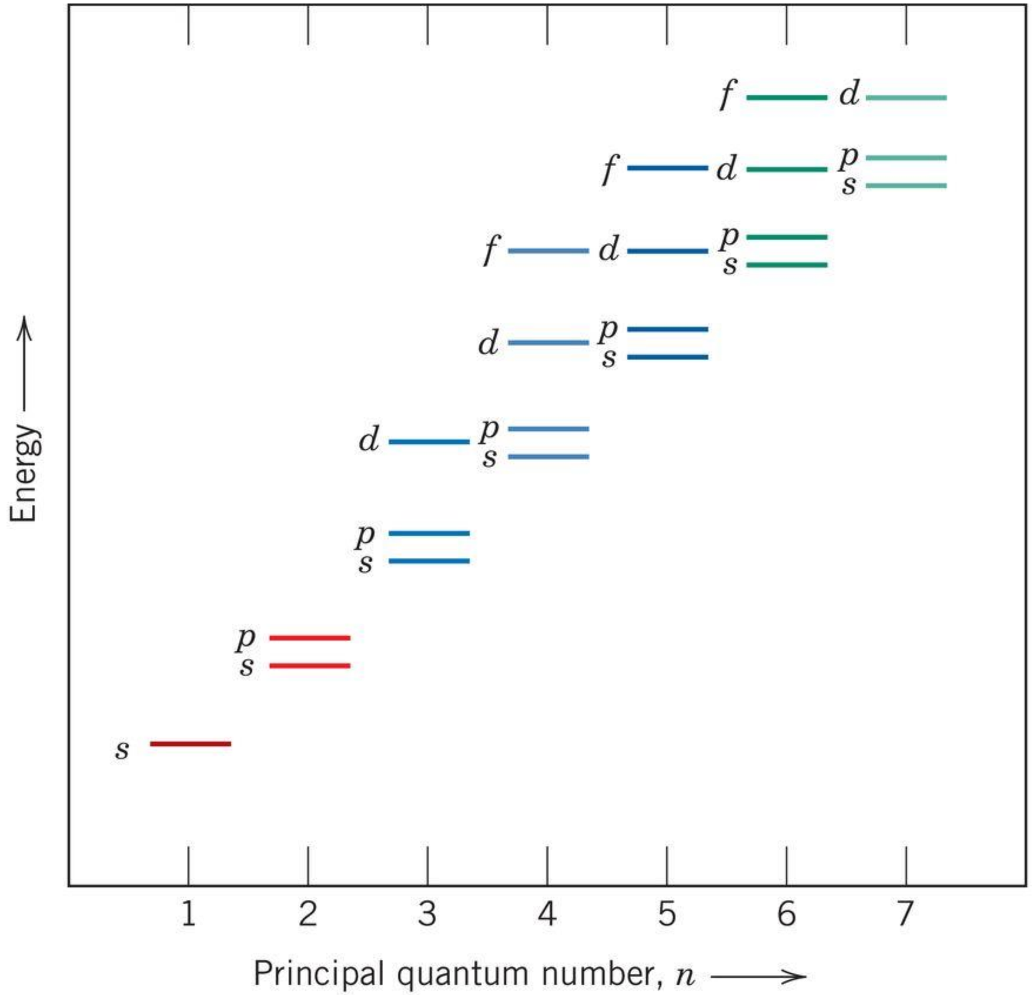




electronic configuration of Na

AN 11





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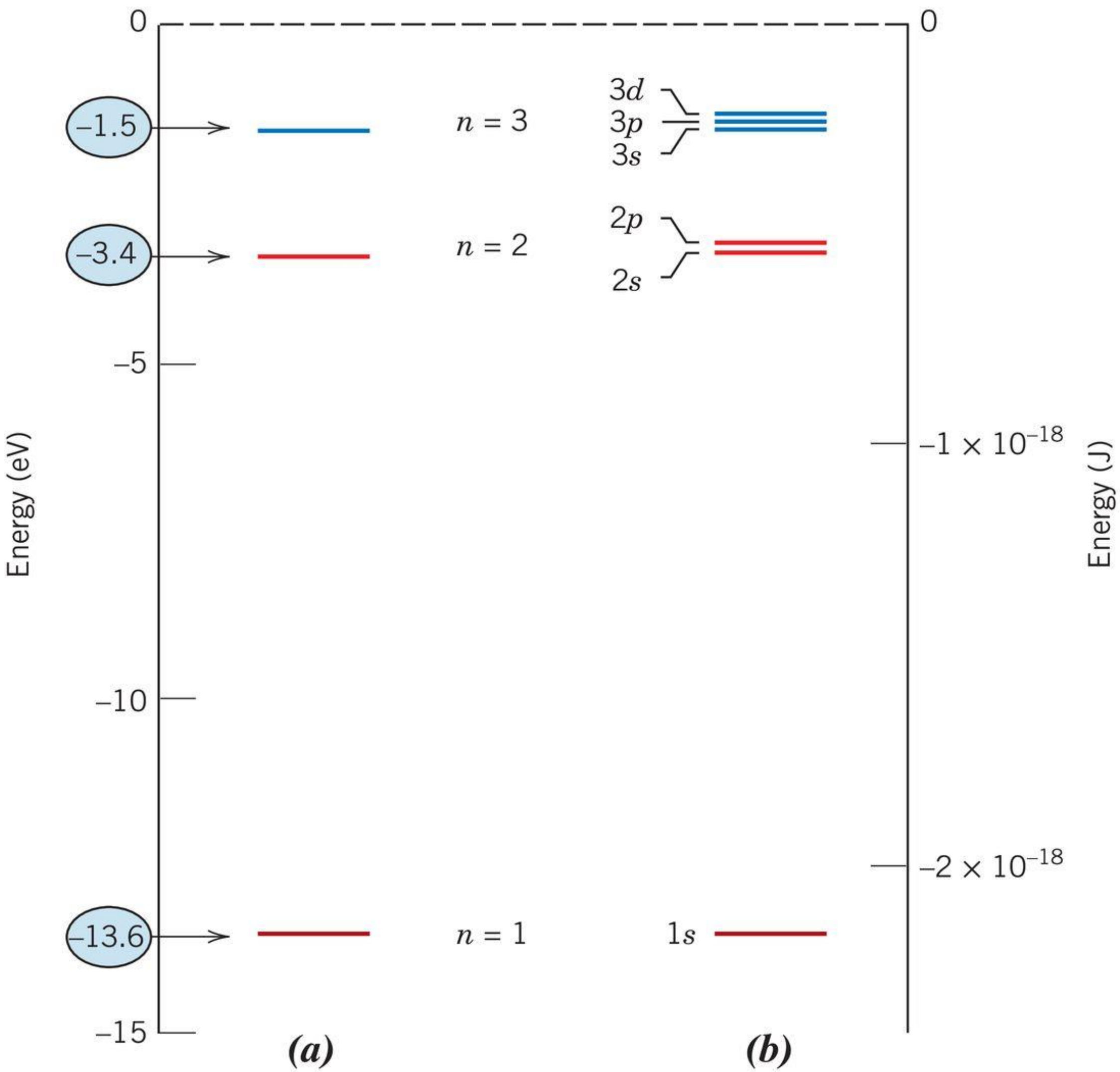

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