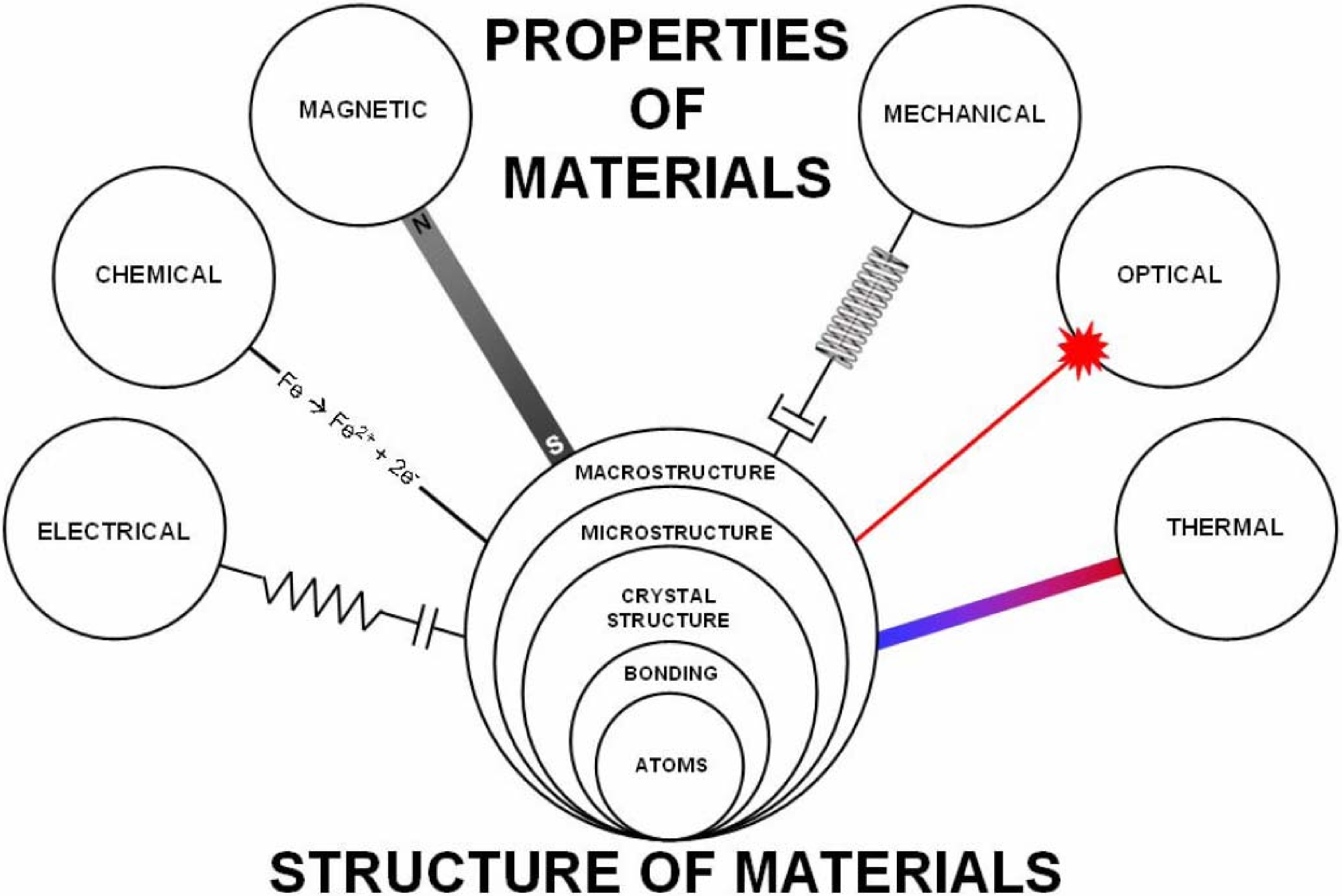
Announcements

- Room change for Tutorial B, Thursdays
  - NOW Trottier 0060 Thursday
- Problems to work on and study from Callister
  - **Ch. 2:** 2.5, 2.6, 2.7, 2.9, 2.11, 2.13, **2.15**, 2.18, 2.20, 2.21, 2.22
  - **Ch. 3 (1st batch):** 3.1, 3.2, 3.5, 3.6, 3.7, 3.10
- Updated course syllabus on WebCT
  - New TA Andreas Klinter

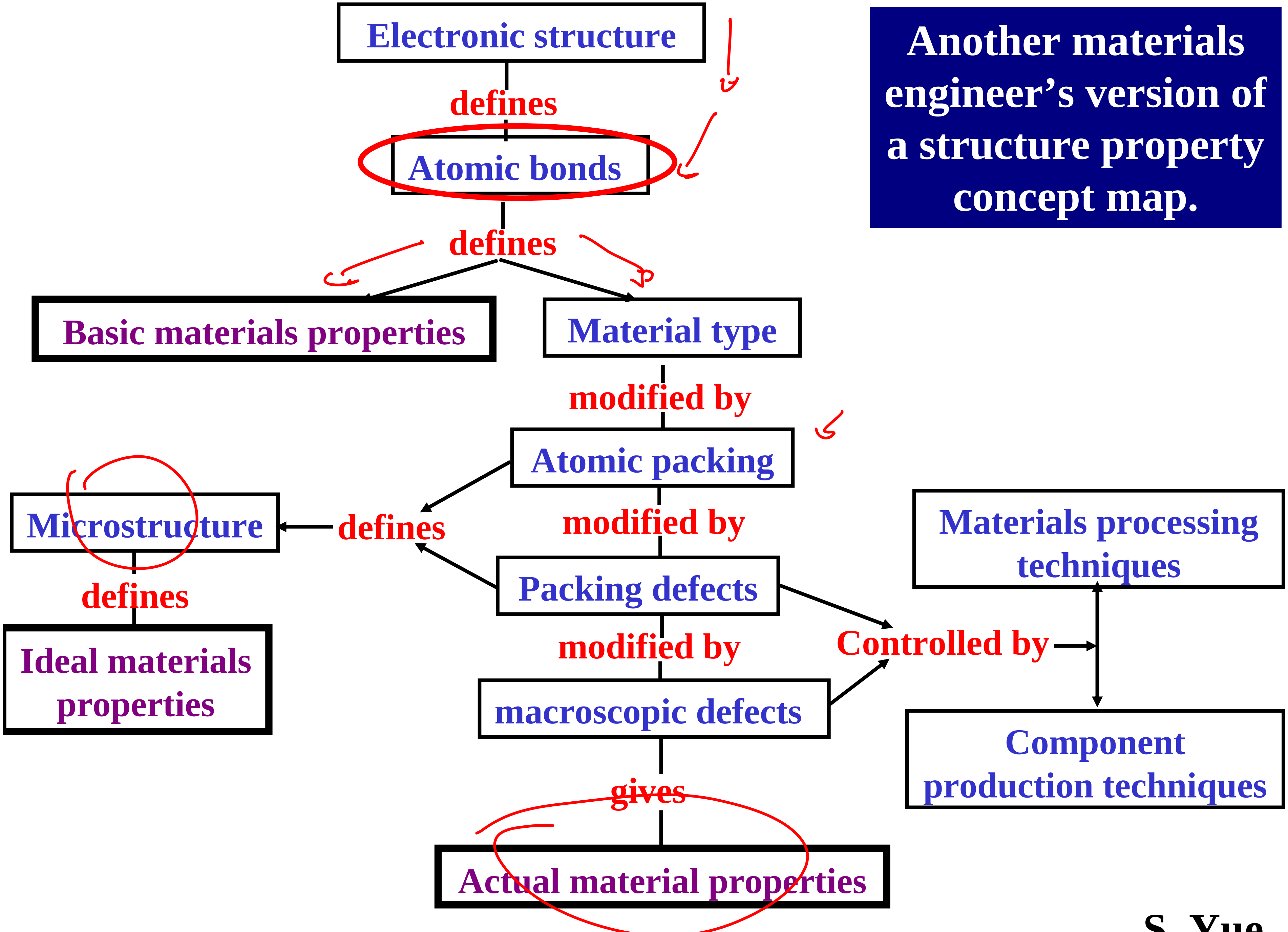
TODAY

- All about bonding

- Start crystal structures


PROPERTIES
OF
MATERIALS
MAGNETIC
MECHANICAL
CHEMICAL
OPTICAL
ELECTRICAL
THERMAL
N
S
Fe → Fe2+ + 2e-
MACROSTRUCTURE
MICROSTRUCTURE
CRYSTAL
STRUCTURE
BONDING
ATOMS
STRUCTURE OF MATERIALS

Another materials engineer's version of a structure property concept map.



S. Yue

BASICS OF ATOMIC BONDING

WHY WOULD ATOMS BOND?

HOW DO ATOMS BOND ?

BASICS OF ATOMIC BONDING

WHY WOULD ATOMS BOND?

KEY CONCEPT

MINIMISATION OF 'ENERGY'

-individual atoms have energy

-atoms bond as a result of lowering total energy of atoms

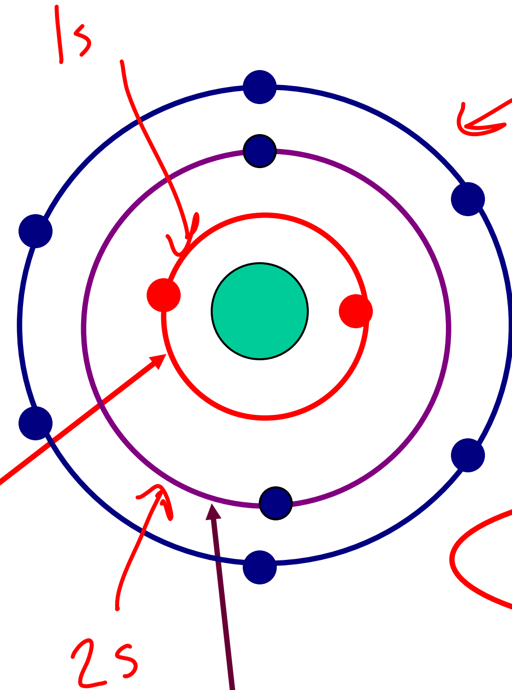
-lowest energy state of an atom =

Ground state

-ground state achieved when all electron shells are filled* in order of increasing energy

~~Therefore, to bond atoms:~~

Usually



'The inert* gases'

outermost shell filled* last

Ne (8), Ar(8), Kr (8) and He (2),

have outermost s and p orbitals full:

"stable electron configuration"

Innermost shell filled first

Then next to innermost shell filled next etc.

For most other elements:

attaining the stable electron configuration……

….leads to atomic bonding

INTERIM SUMMARY

-individual atoms have energy

-atoms bond as a result of lowering total energy of atoms

-lowest energy state of an INDIVIDUAL atom = Ground state

- lowest energy state of A GROUP OF atoms = stable electron configuration*

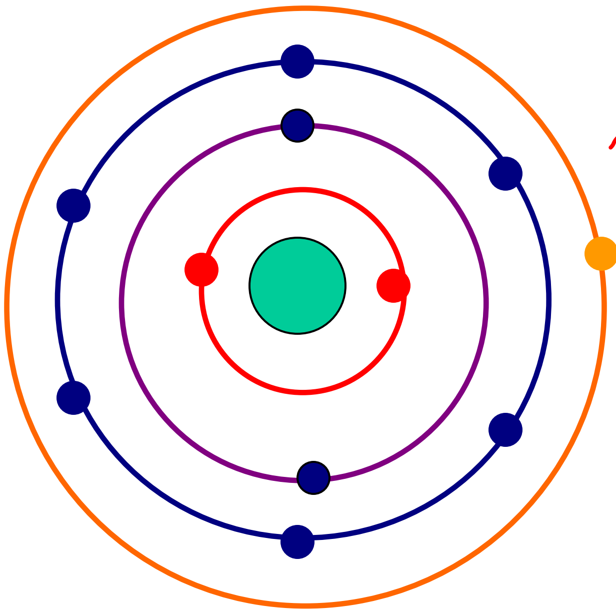
Therefore, to bond atoms:

Attain stable electron configuration….

……………..by filling all the shells

e.g. recall 6 electrons fills **third** subshell 2p

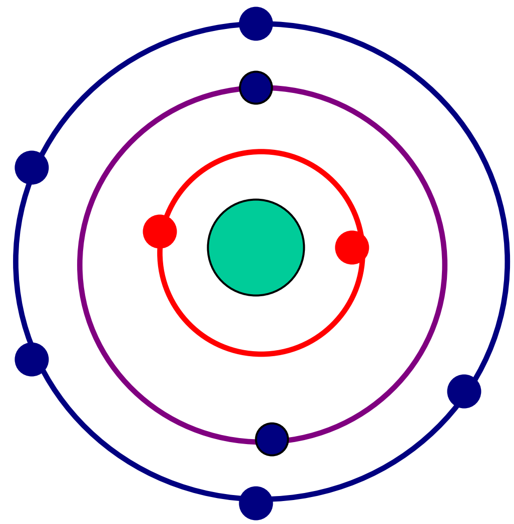
Element A



3s

+

Element B



−

Small excess of electrons
metallic, or electropositive

Small deficiency of electrons
non-metallic or $\boxed{\text{electronegative}}$

Losing an electron…..

OR

gaining an electron…..

Leads to stable electron configuration

And bonding

PERIODIC TABLE*

Lose e^-

Gain e^-

	IIA	IIIB	IVB	VB	VIB	VIIB	VIII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	
1 H 2.1																	2 He —
3 Li 1.0	4 Be 1.5											5 B 2.0	6 C 2.5	7 N 3.0	8 O 3.5	9 F 4.0	10 Ne —
11 Na 0.9	12 Mg 1.2											13 Al 1.5	14 Si 1.8	15 P 2.1	16 S 2.5	17 Cl 3.0	18 Ar —
19 K 0.8	20 Ca 1.0	21 Sc 1.3	22 Ti 1.5	23 V 1.6	24 Cr 1.6	25 Mn 1.5	26 Fe 1.8	27 Co 1.8	28 Ni 1.8	29 Cu 1.9	30 Zn 1.6	31 Ga 1.6	32 Ge 1.8	33 As 2.0	34 Se 2.4	35 Br 2.8	36 Kr —
37 Rb 0.8	38 Sr 1.0	39 Y 1.2	40 Zr 1.4	41 Nb 1.6	42 Mo 1.8	43 Tc 1.9	44 Ru 2.2	45 Rh 2.2	46 Pd 2.2	47 Ag 1.9	48 Cd 1.7	49 In 1.7	50 Sn 1.8	51 Sb 1.9	52 Te 2.1	53 I 2.5	54 Xe —
55 Cs 0.7	56 Ba 0.9	57–71 La–Lu 1.1–1.2	72 Hf 1.3	73 Ta 1.5	74 W 1.7	75 Re 1.9	76 Os 2.2	77 Ir 2.2	78 Pt 2.2	79 Au 2.4	80 Hg 1.9	81 Tl 1.8	82 Pb 1.8	83 Bi 1.9	84 Po 2.0	85 At 2.2	86 Rn —
87 Fr 0.7	88 Ra 0.9	89–102 Ac–No 1.1–1.7															

Z

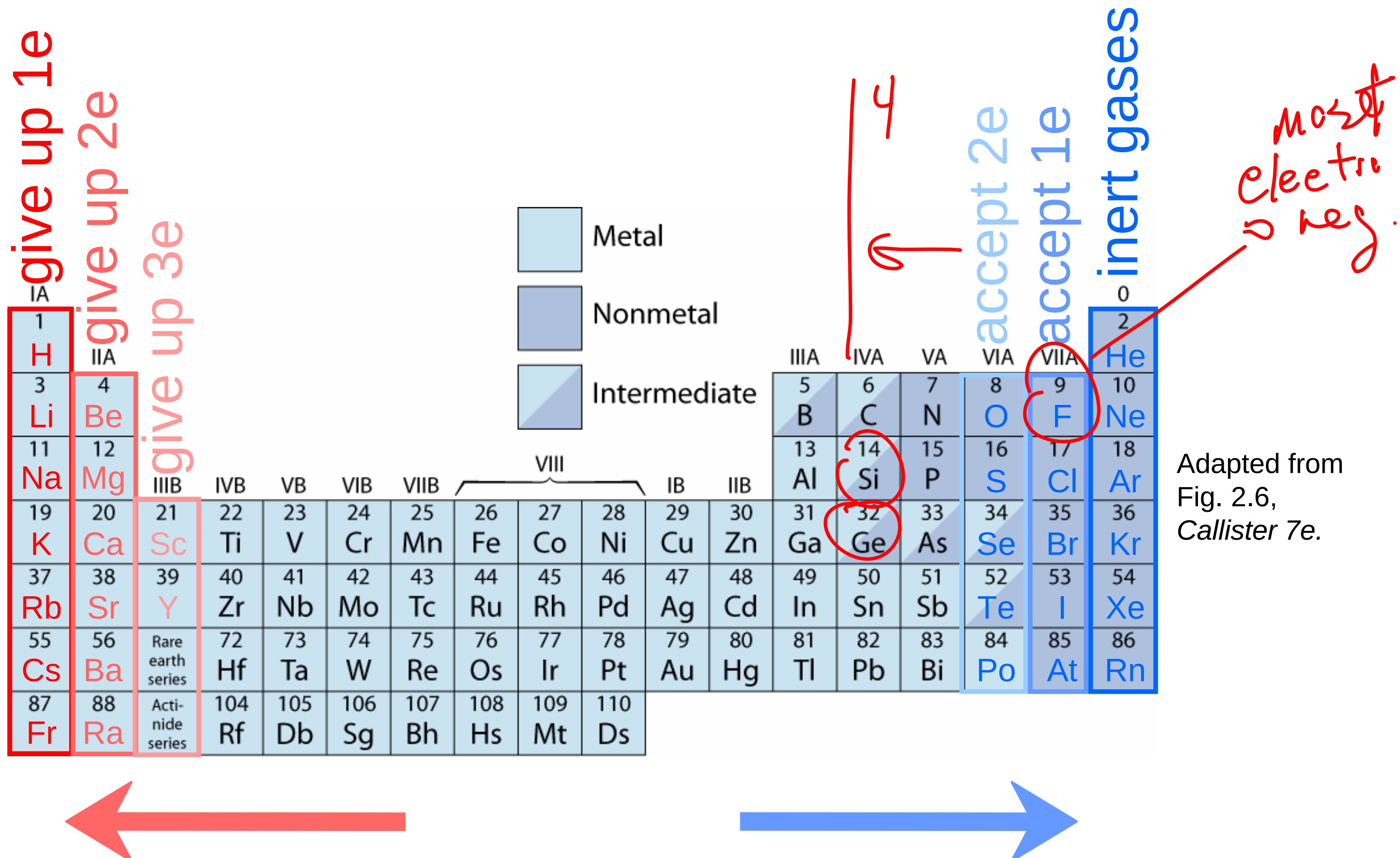
Increasing electropositivity

Z

Increasing electronegativity

The Periodic Table

- Columns: Similar Valence Structure



Adapted from Fig. 2.6, *Callister 7e.*

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

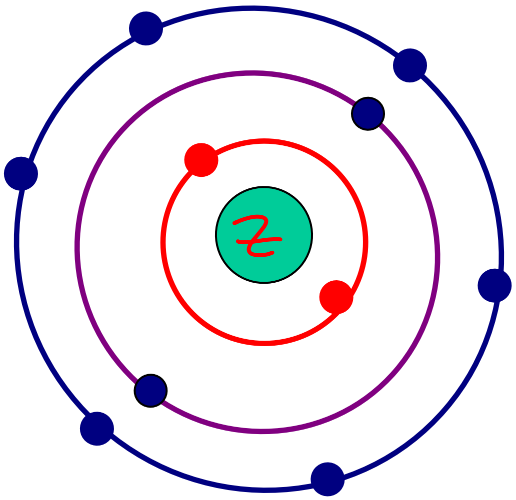
Electronegative elements:
Readily acquire electrons
to become - ions.

ATOMIC BONDING (HOW..?)

PRIMARY BOND TYPES "STRONG"

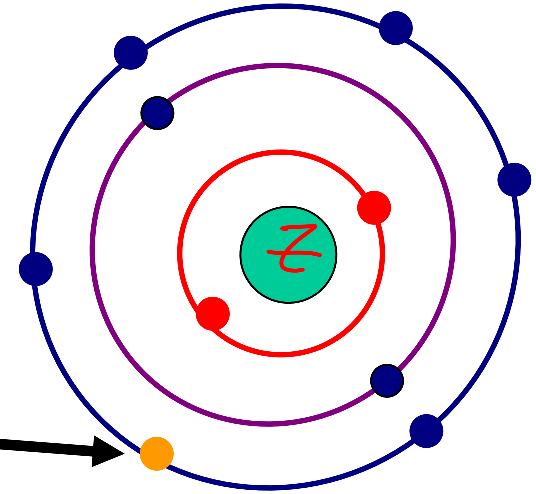
IONIC **big difference in electronegativities**

Element A



To attain stable electron configuration

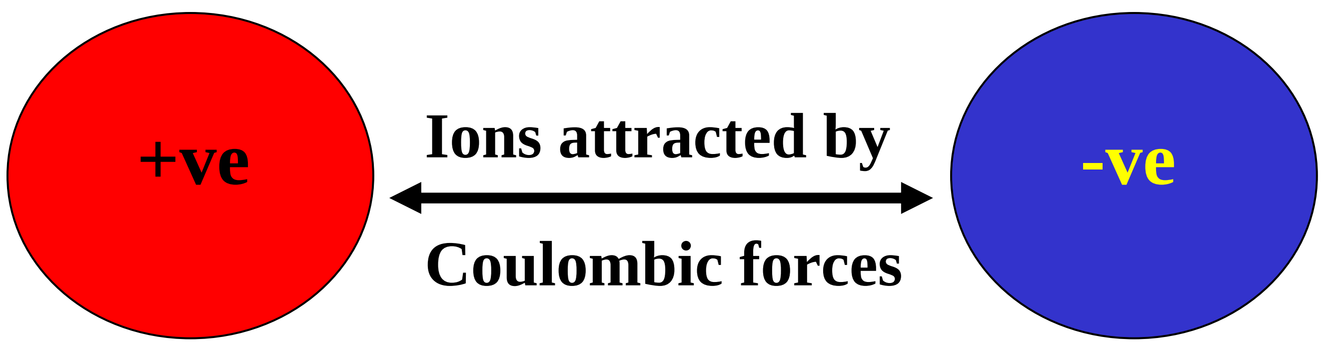
Element B



Metal gives electron to non metal

transfer e^-

+1 −1

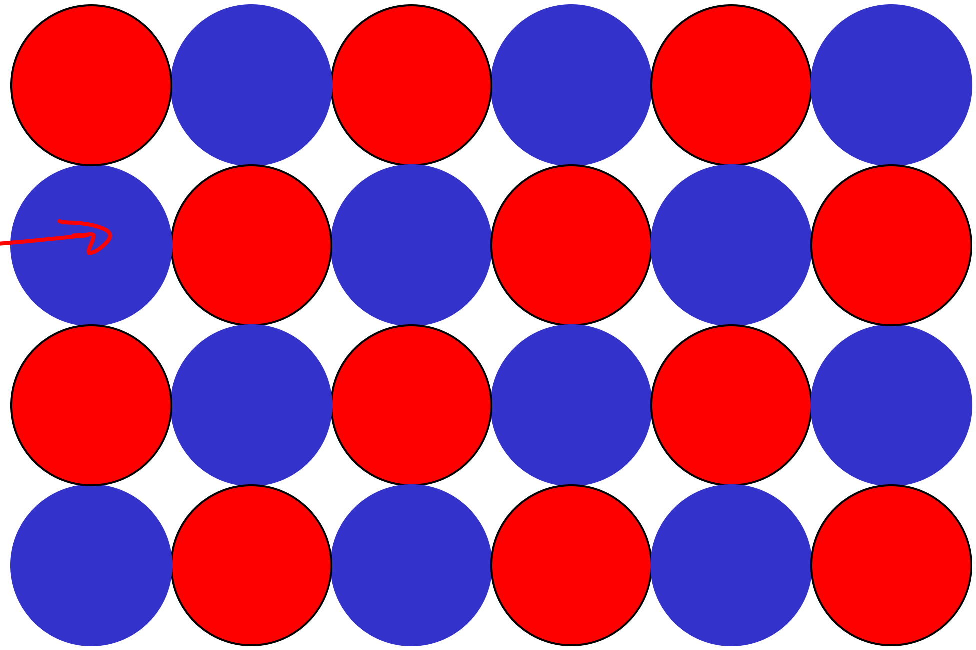


Ions attracted by Coulombic forces

Forces are non-directional (or omni-directional)

Therefore,

red



i.e. nearest neighbours of +ve (-ve) ions are -ve (+ve) ions

large molecules can be formed in 3D $NaCl$

CERAMICS bonded in this way Al_2O_3

NaCl forms

EXAMPLE

	IIA	IIIB	IVB	VB	VIB	VIIB	VIII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	
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87 Fr 0.7	88 Ra 0.9	89–102 Ac–No 1.1–1.7															

Na
Needs to lose one electron

Cl
Needs to gain electron

K
Loses 1 electron

Ca Gains 16 electrons?

i.e. ionic bonding only when electronegativities are ‘far’ apart

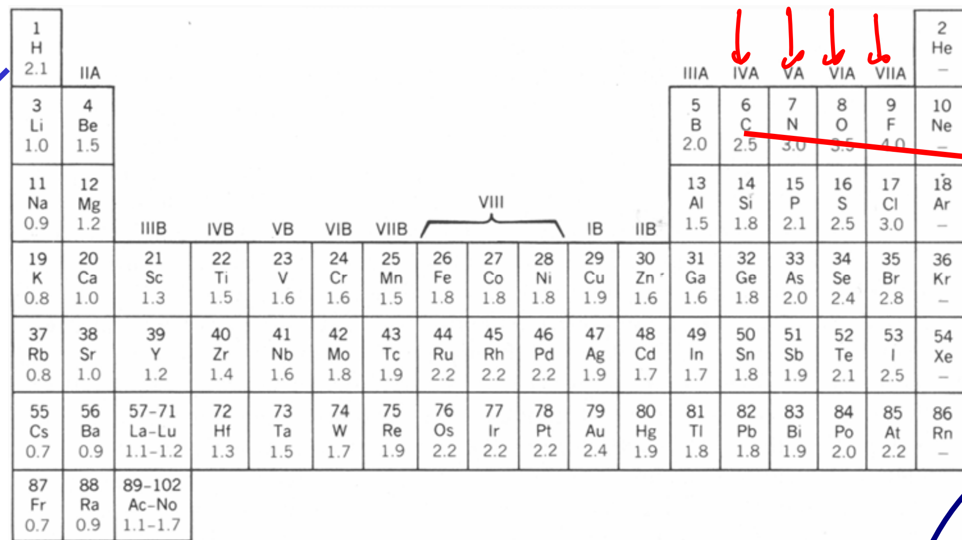
Otherwise, electrons are shared

COVALENT BONDING

electronegative elements 4 or more valence electrons

and H

4



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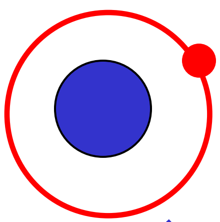
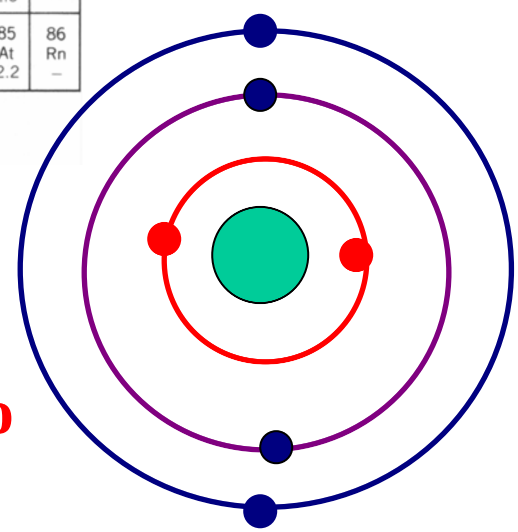
87 Fr 0.7	88 Ra 0.9	89–102 Ac–No 1.1–1.7															

C

H



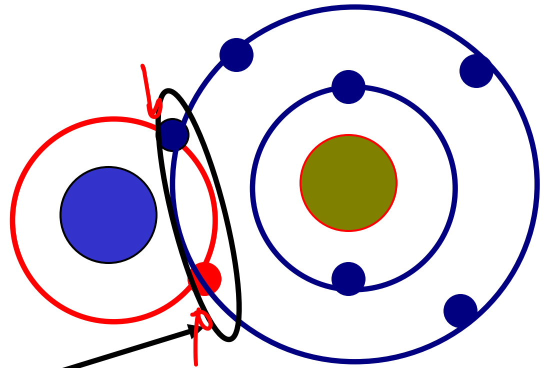
Needs to gain one electron



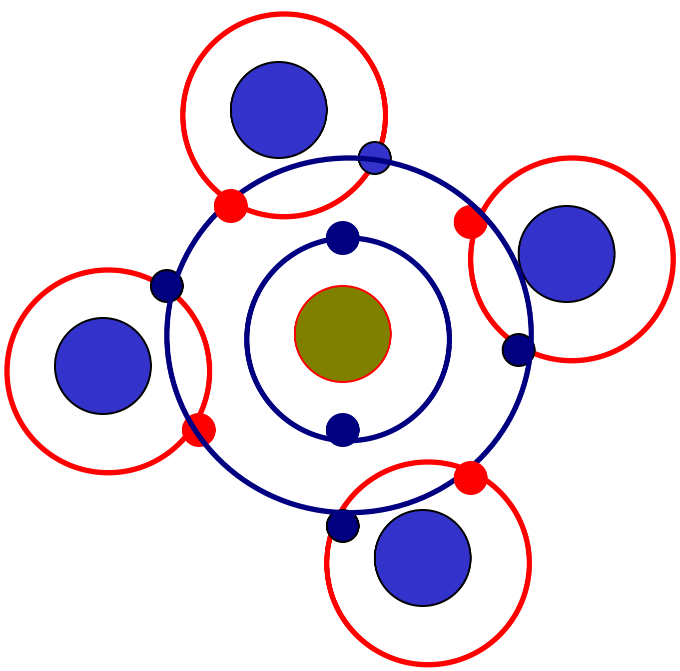
Needs to gain 4 electrons

H and C 'gain' each others electron by sharing electrons

Electron 'cloud' attracts nuclei



Hydrogen now is at ground state: C needs 3 more electrons



Obtained by sharing with three more H atoms

CH_4

Covalent bonds are directional

Non-metallics (electronegatives) have this bond

(elemental or compounds)

e.g. ceramics, plastics

Many compounds have a mixture of covalent and ionic

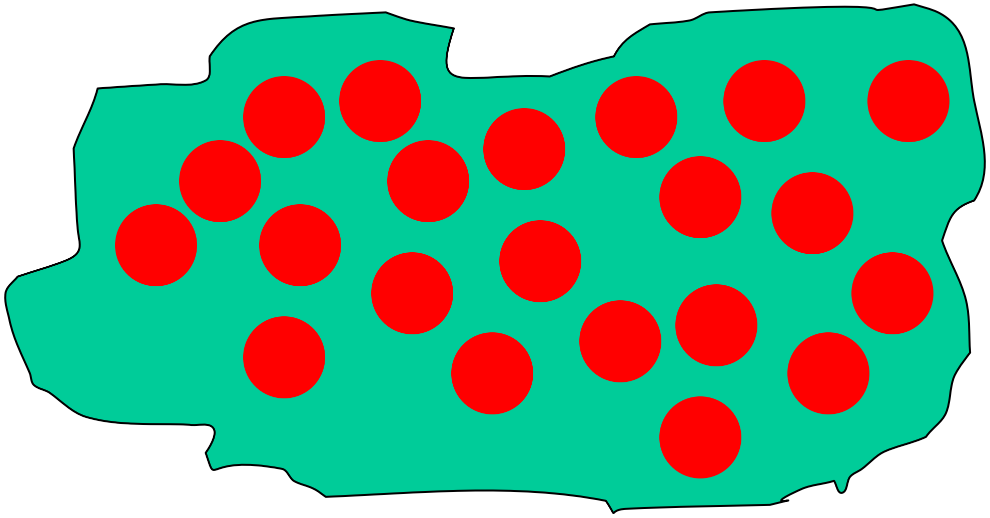
Increasing difference in electronegativity = increasing ionic 'character' in compounds

Metallic bonds

All valence electrons freed up to form electron ‘cloud’

All atoms share all electrons in cloud

each atom reaches lower energy state



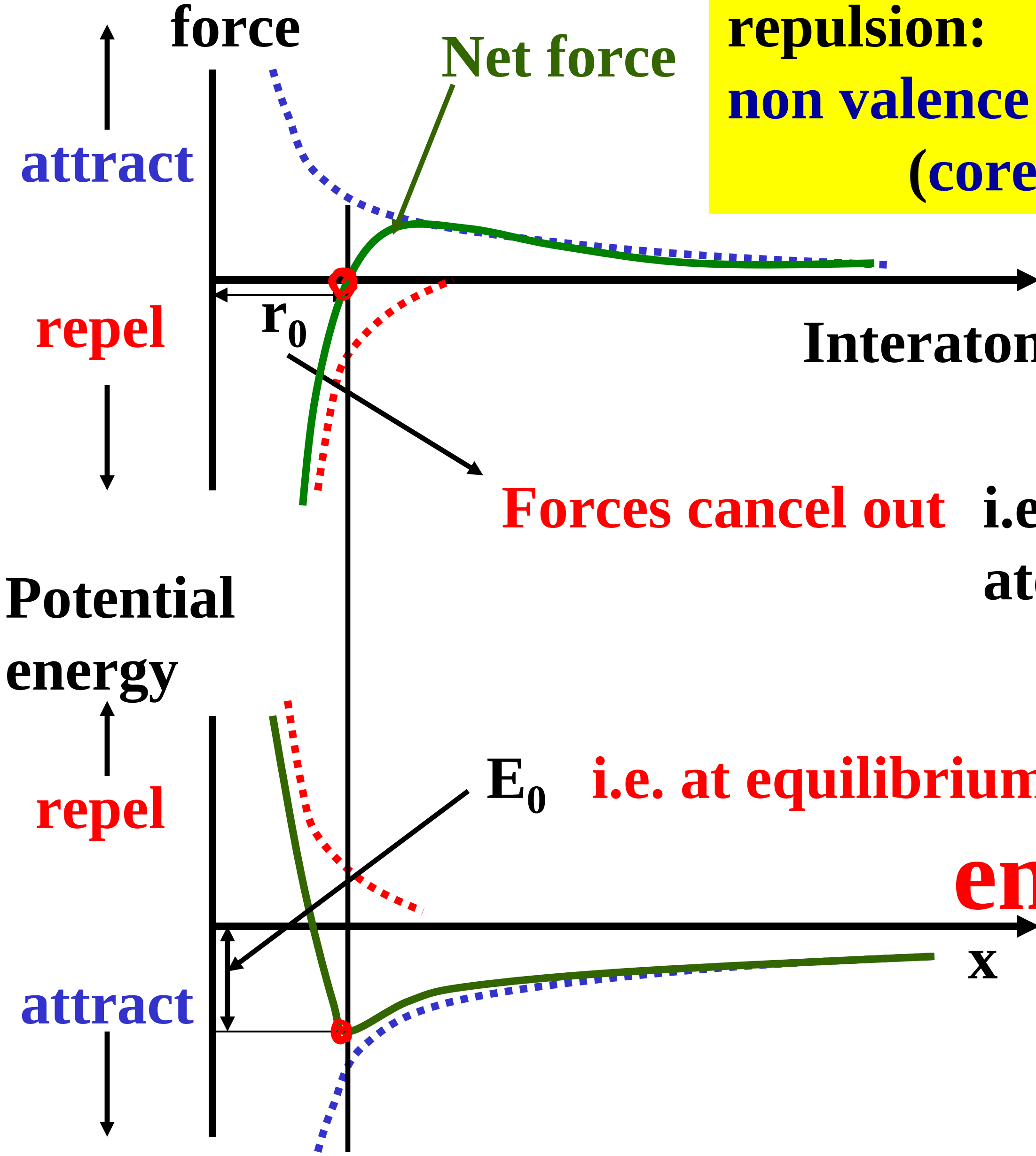
Cloud attracts metal ions (ion ‘cores’)

Non-directional forces, therefore close packed

Forces can be weak or strong
(melting points vary by 1000s of degrees)

BONDING FORCES AND ENERGY

repulsion:
non valence electrons interact (core electrons)



$$F = \frac{-\partial U}{\partial r}$$

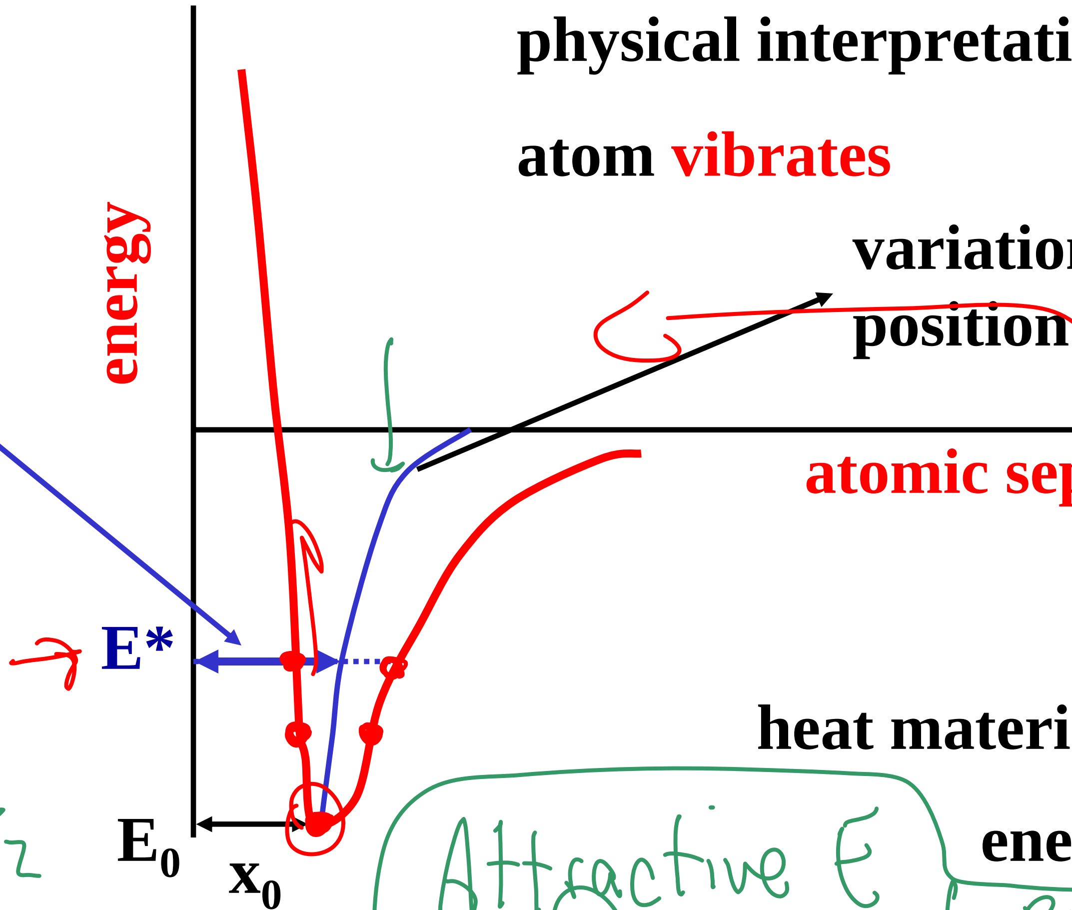
Forces cancel out i.e. **equilibrium atomic separation**

i.e. at equilibrium atomic separation

energy lowest

RELATION BETWEEN ATOMIC BONDING AND THERMAL EXPANSION

$$\frac{x_e - x_0}{x_0}$$



atomic separation = r

physical interpretation?

atom vibrates

variation of mean position with temp

heat material = energy increase

Lennard Jones

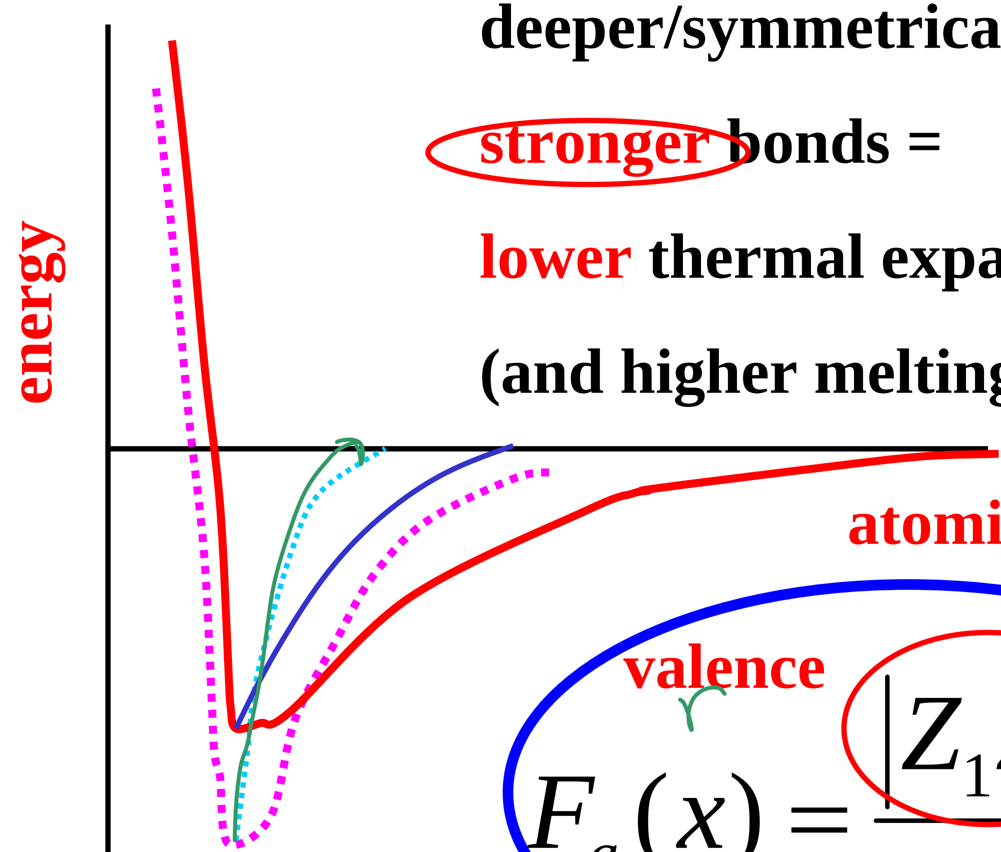
Attractive E $-A/r$

Repulsive E B/r^n

x

r^6 r^{12}

RELATION BETWEEN ATOMIC BONDING AND THERMAL EXPANSION



deeper/symmetrical curve =

stronger bonds =

lower thermal expansion

(and higher melting points)

atomic separation

valence

$$F_a(x) = \frac{|Z_1 Z_2| q^2}{4\pi\varepsilon_0 x^2}$$

electron charge

capacity of a material to be polarized by an electric field

permettivity of vacuum

F(x)

IONIC

Equation explanation
Coulombic force between two ions

$$F_a(r) = \frac{|Z_1 Z_2| q^2}{4\pi\varepsilon_0 r^2}$$

q – charge on one electron

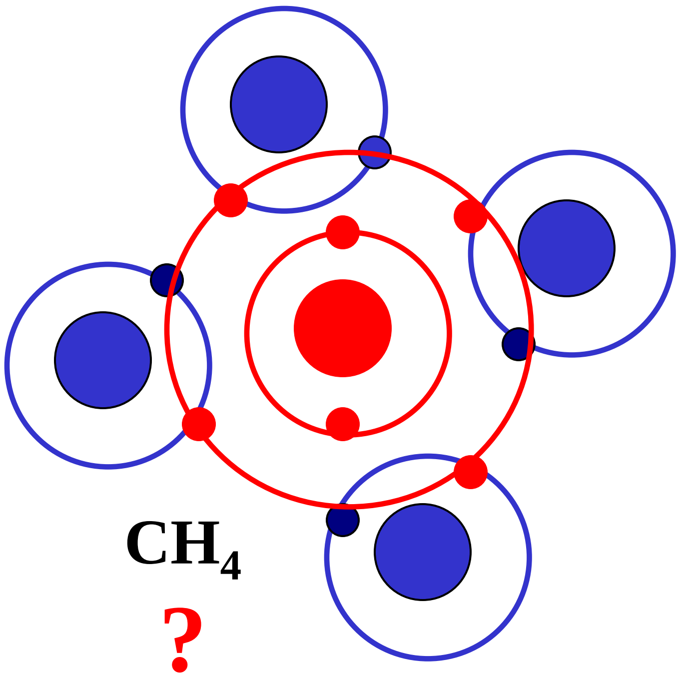
Z_1 and Z_2 – valence (NOT atomic number in this case) Example Na bonds with Cl. Valence of Na^+ is +1 and Cl^- is -1.

r – interatomic separation

ε_o – permittivity of vacuum

COVALENT

QUESTION



Methane is a gas because

-all atoms are at ground state

-coulombic forces are directional

BUT*

Methane condenses and solidifies at very low temperatures.

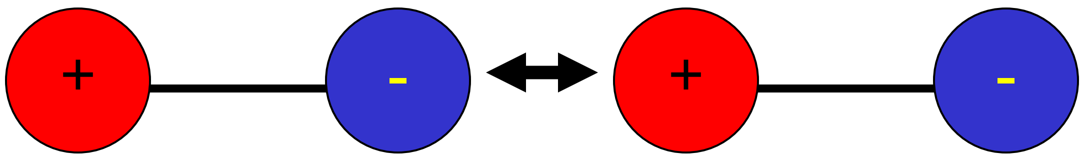
i.e. molecules are bonding

HOW DO THE MOLECULES BOND?

Secondary Bond "Weak"

SECONDARY OR
VAN DER WAALS BONDING

If there is any separation of electrons and protons:



'dipole' is formed **Attracts other dipoles**

Dipoles occur frequently

But usually obscured by primary bonds

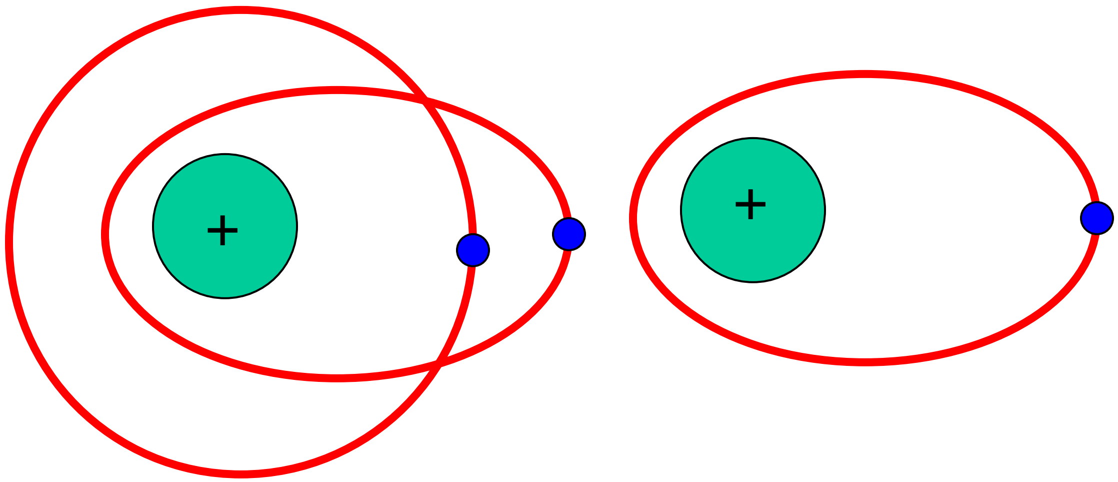
Dipoles bond molecules (or atoms) in which all valence orbitals are filled

IMPORTANT FOR PLASTICS

DIPOLE FORMATION

Fluctuating induced dipoles

Temporary distortion of symmetrical atom due to general atomic vibrations.



dipole forms **Attracts other dipoles**

Effect of low temperatures:

Slows down movement of atoms

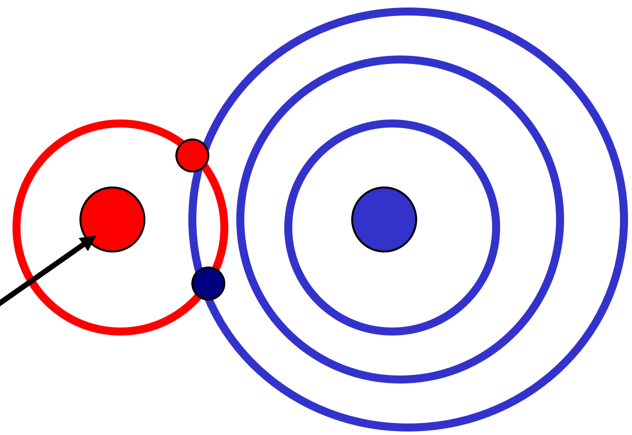
increases probability of interaction

Condenses (liquefaction) inert gases: weakest bonds…..

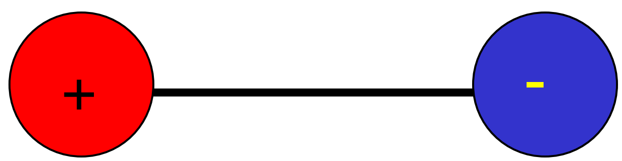
PERMANENT DIPOLE BONDS

Asymmetric molecules

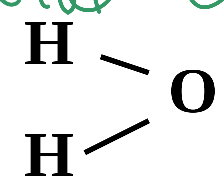
H: special case



Proton unshielded on one side
Creates hydrogen bond
e.g. water



special case of dipole bond



SUMMARY

- Types of bonding
  - ‘Strong’ bonds: covalent, ionic and metallic
  - ‘Weak’ bonds: van der Waals and dipole (hydrogen)
- Which bond type depends on what is bonding (e.g. groups of atoms find most stable electron configuration)

WHY?

Bond Energies

Bonding Type	Substance	Bonding Energy kJ/mol	Bonding Energy eV/Atom, Ion, Molecule	Melting Temperature (°C)
Ionic	NaCl	640	3.3	801
	MgO	1000	5.2	2800
Covalent	Si	450	4.7	1410
	C (diamond)	713	7.4	>3550
Metallic	Hg	68	0.7	−39
	Al	324	3.4	660
	Fe	406	4.2	1538
	W	849	8.8	3410
van der Waals	Ar	7.7	0.08	−189
	Cl_2	31	0.32	−101
Hydrogen	NH_3	35	0.36	−78
	H_2O	51	0.52	0

Ionic bonds are generally the strongest. But, as you can see here, the bond energy varies: (1) from type-to-type, (2) within each bond type.