Material classes and atomic bonding

What holds everything together?

41680 Introduction to advanced materials

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Department of Civil and Mechanical Engineering

You’re a mechanic, right? Why don’t you just build something?

Kid to Tony Stark in Iron Man 3

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Material classes - properties

Polymers

Metals

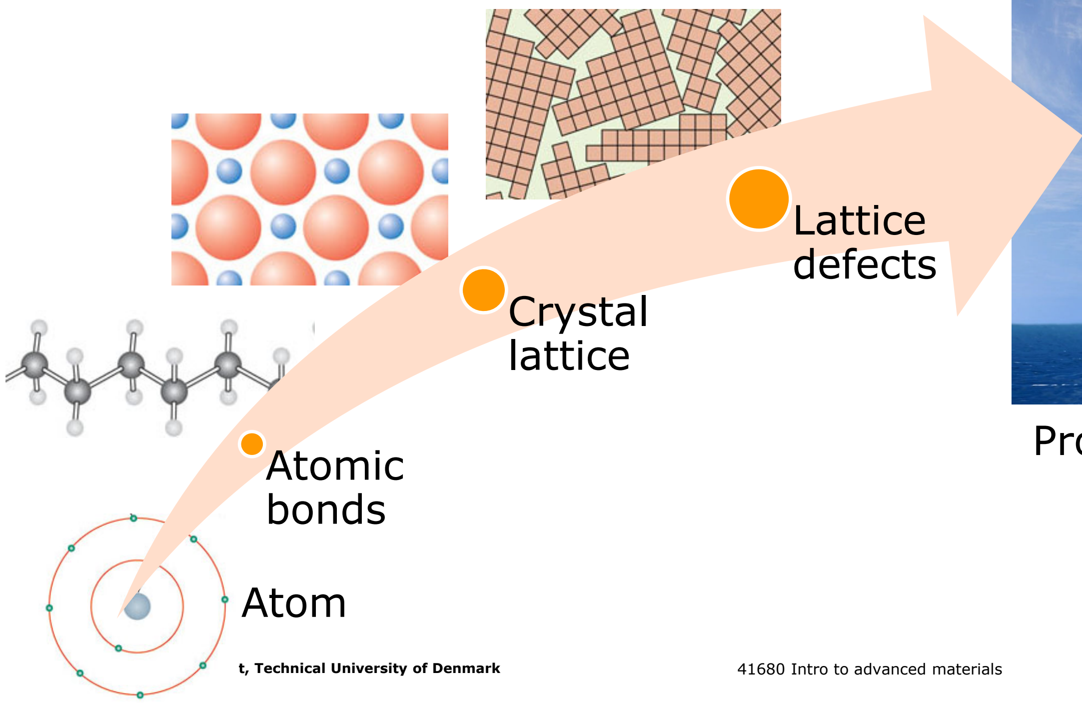
Ceramics

Group exercise
Material classes (Pros and Cons)

Class	Metals	Ceramics	Polymers
Pros	Group 1	Group 2	Group 3
Cons			

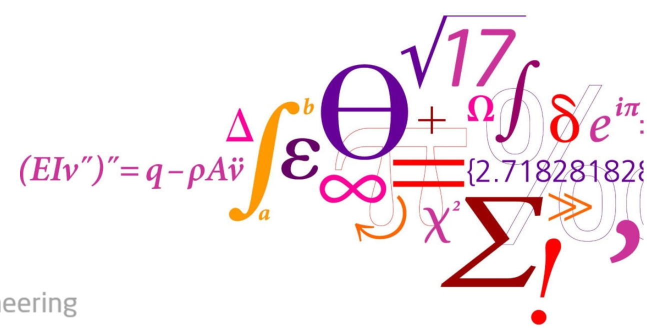
Discuss the advantages and disadvantages of using materials from the different classes in groups. Present the findings of your assigned task in plenum, e.g. group 2 should summarise advantages and disadvantages of ceramics

Advanced materials
Atoms - Microstructure - Properties



Product

Atomic bonds (in solids)



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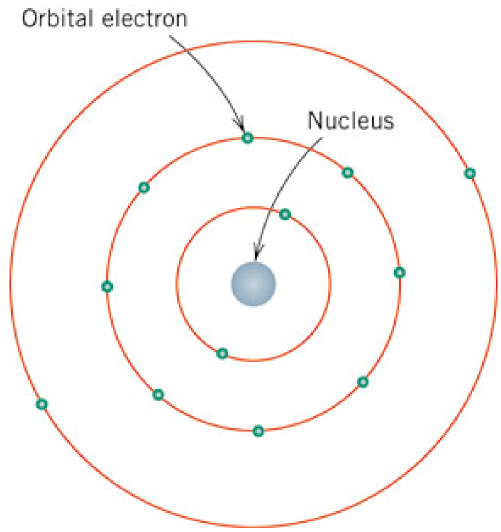
Bohr's model of the atom (1913)



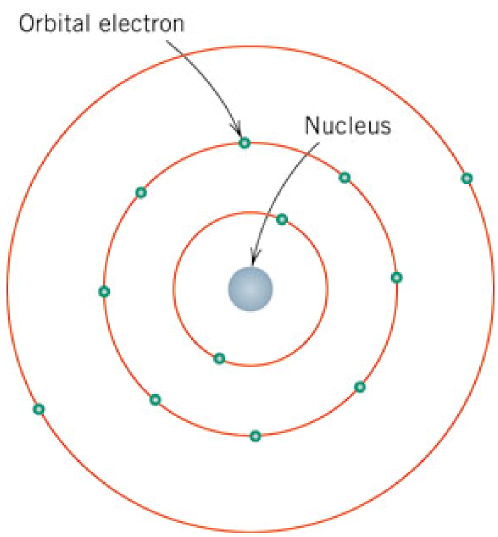
- Nucleus
  - protons
  - neutrons
- Electrons
  - discrete tracks
  - discrete energy levels
  - electron shells
- Periodic system of elements
  - Order according to number of protons

Periodic system of elements (June 2016)

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	*L*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	*A*	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og
		L	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
		A	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

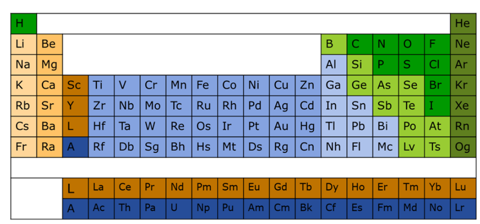
Alkali metals	Actinides	Metalloids
Alkaline earth metals	Transition metals	Non-metals
Lanthanides	Other metals	Noble gases

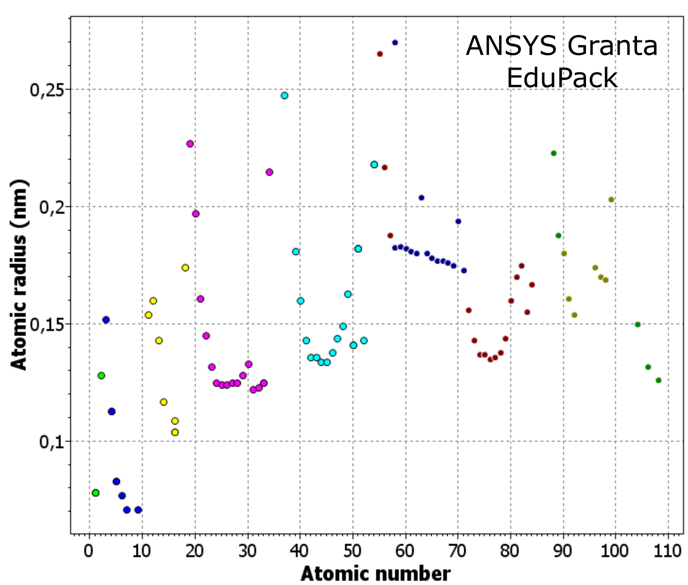
Bohr’s model of the atom (1913)



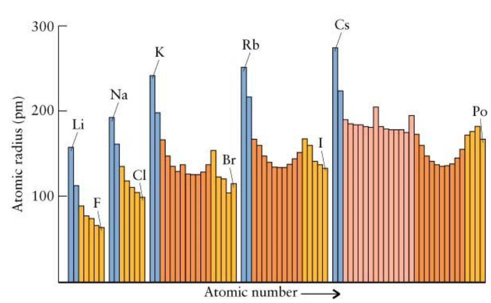
- Nucleus
  - protons
  - neutrons
- Electrons
  - discrete tracks
  - discrete energy levels
  - electron shells
  - stable configuration of the noble gases
  - octet rule
  - inner electrons
  - valence electrons

Atomic radius – periodic variation





Atomic radius / pm



Electronegativity X (Pauling) F24

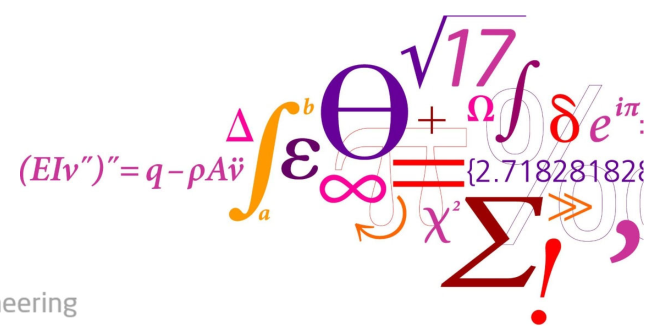
- Tendency to attract and bond electrons

IA	IIA	IIIB	IVB	VB	VIB	VIIB	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															

Lower electronegativity
(donates electrons)

Higher electronegativity
(accepts electrons)

Interatomic forces



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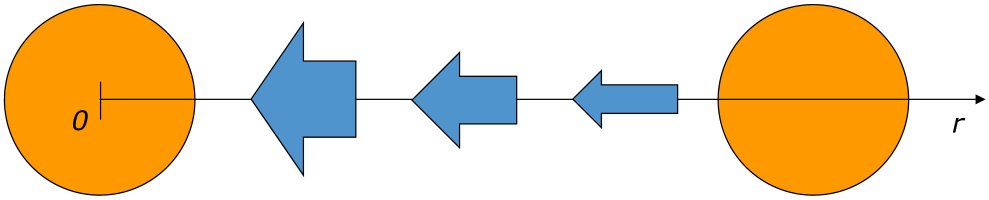
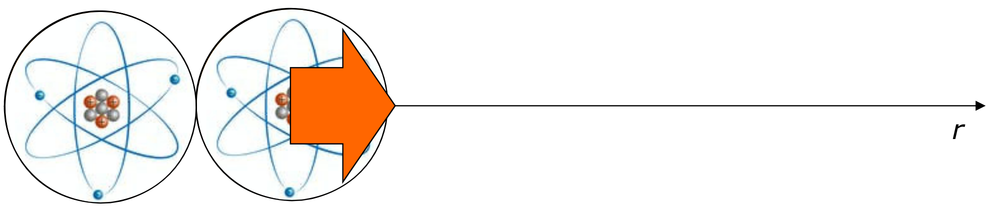
Interatomic forces

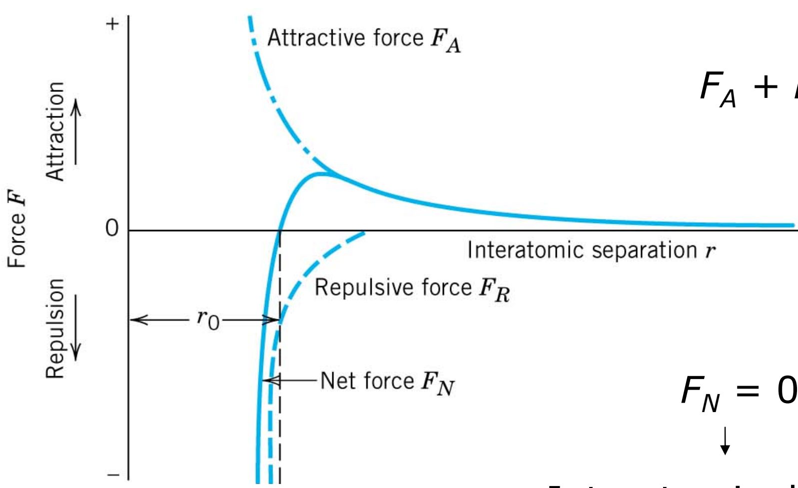
- Attraction (the stronger, the closer)



- Repulsion



Bonding forces between atoms



$$F_A + F_R = F_N$$

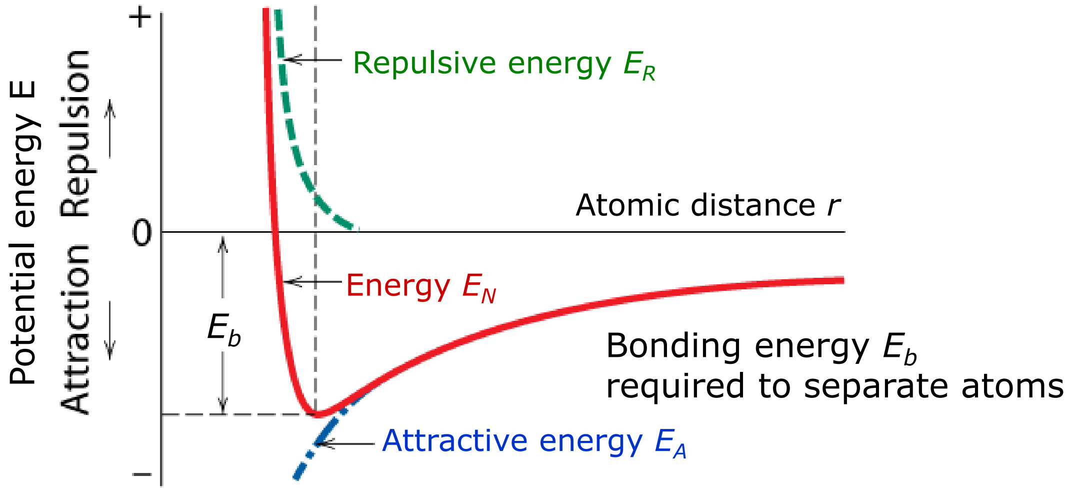
$$F_N = 0$$

↓

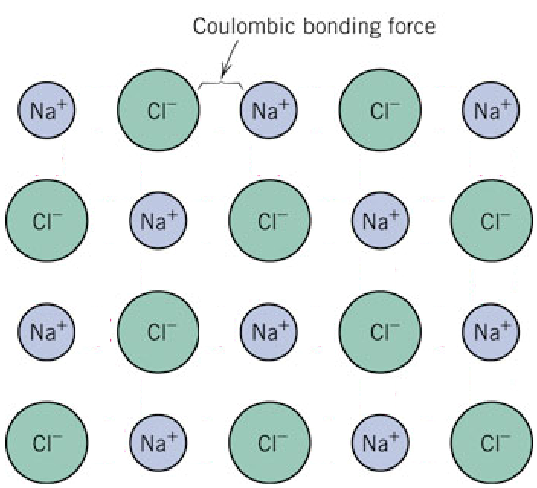
Interatomic distance r_0

(equilibrium distance between atoms)

Bonding energy



Ionic bonding

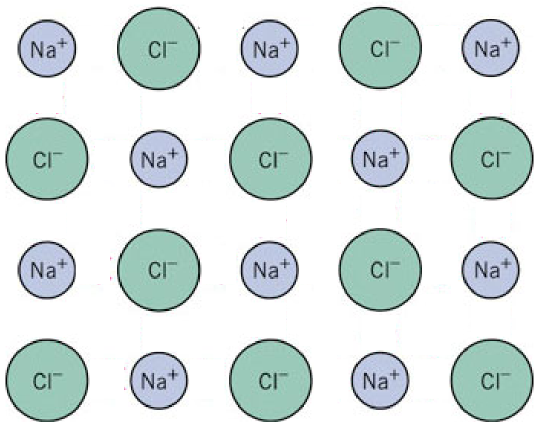


- Metal + Non-metal
- Low + high electronegativity
- Complete transfer of electron

$$Na + Cl \rightarrow Na^{+} + Cl^{-}$$

- Atoms become ions with electrical charge
- Coulomb forces
  - Long range
- Bond
  - Without direction
  - Many neighbors

Ionic bonding



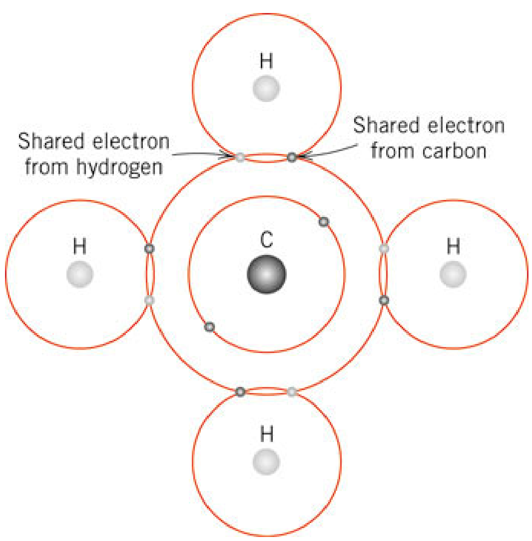
Examples

- Salt (NaCl)
- Minerals (Al_2O_3)
- Classical ceramics (SiO_2)
- Technical ceramics (MgO)

Consequences

- Low electric conductivity (DC)
- Brittle

Covalent bonding / electron pair bonding



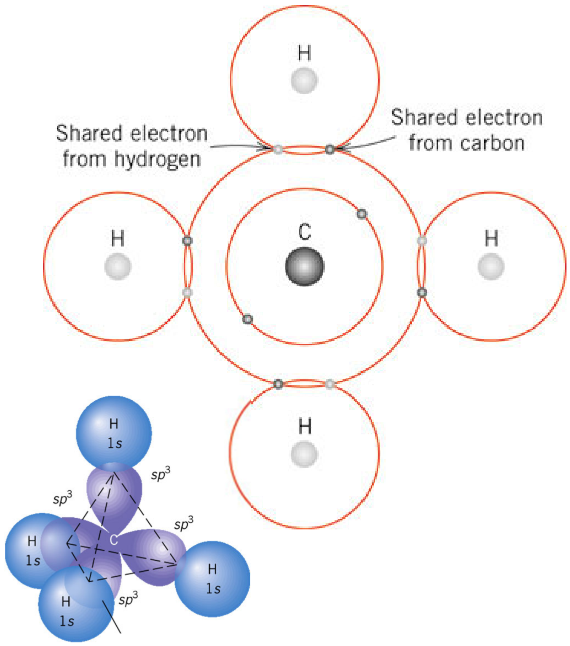
- Non-metal + Non-metal (or metalloids)
- Octet rule
- Two atoms share electron pairs

Covalent bonding

- With direction
- Only immediate neighbor
- Valence = number of possible bonds

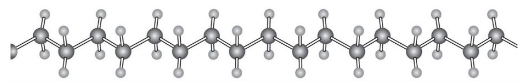
n **valence electrons**	**Number of bonds**
$n \le 4$	n
$n \ge 4$	$8 - n \quad (n)$

Covalent bonding / electron pair bonding



Examples

- Molecules (H_2, N_2, H_2O, CH_4)
- Solid elements (Si, diamond)
- Compounds (GaAs, SiC)
- Polymers



Consequences

- Low electrical conductivity
- High thermal conductivity
- Brittle

Covalent bonding / electron pair bonding

Atoms of same kind

- Equally sharing of electron pair

$$\mathrm{H} - \mathrm{H}$$

- Nonpolar bond

Atoms with different electronegativity

- Uneven sharing of electron pair

$$\overset{\delta+}{\mathrm{H}} - \overset{\delta-}{\mathrm{Cl}}$$

- Polar bond
- Small electrical dipole
- Difference in electronegativity

$$\Delta X = X_A - X_B$$

Bond type: ionic vs. covalent

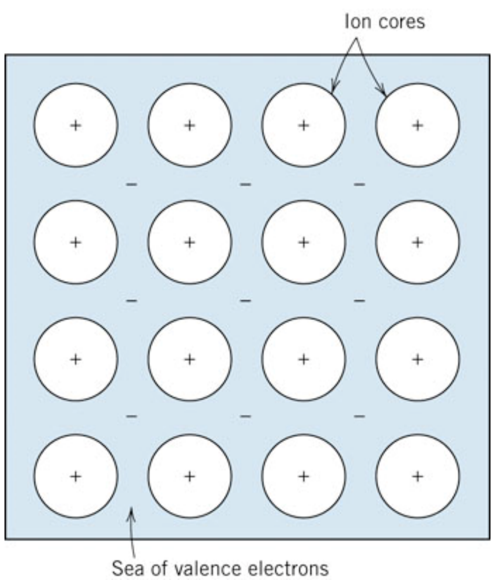
- Bonding between atoms of two elements A and B
- Never pure ionic bonds
- Fraction of ionic bond (empirical relation)

$$f_{Ion} = 1 - \exp\left[-\frac{(X_A - X_B)^2}{4}\right] = 1 - e^{-\frac{(X_A - X_B)^2}{4}}$$

- Electronegativities X_A and X_B
- Fraction valid for bond A-B, not only for compound AB!
- Example: SiO_2 51%

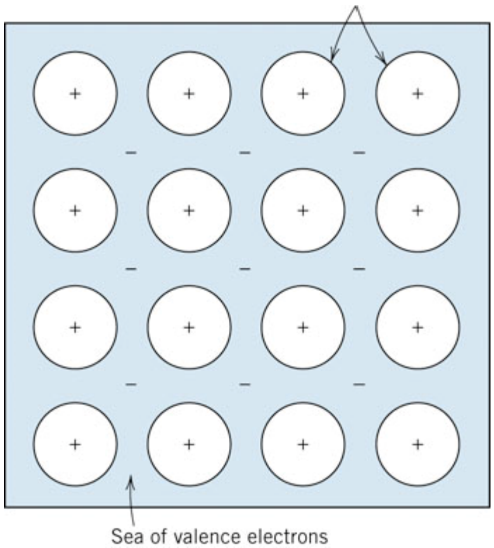
Chemical compound	Ionic fraction
CsCl	73%
NaCl	67%
ZnS	18%

Metallic bonding



- Electrons shared between all atoms
- Valence electrons
  - Do not belong to any atom (free electrons)
  - Electron cloud
  - Conduction electrons
- Bond without direction
  - Long range
- Inner electrons localized
  - (extra covalent bond)
- Positive charge
  - Ions, not nuclei!
  - Many neighbors

Metallic bonding



Examples
- all metallic elements
  (Fe, Al, Cu, Zn)
- alloys
  (brass, bronze)

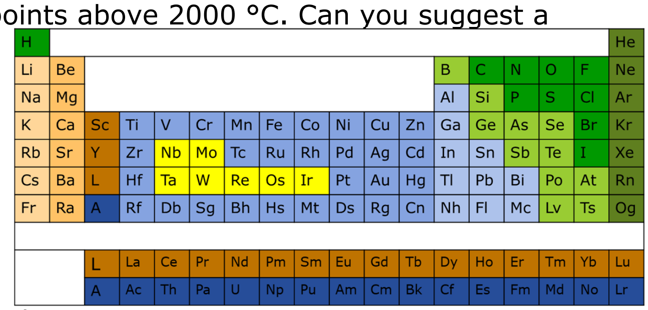
Consequences
- High electric conductivity
- High thermal conductivity
- Reflectivity
- Ductility/Malleability

Group exercise

1. Find the fraction of ionic bonding for different chemical compounds and chemical bonds given by the number N of your breakout room.

Group number N		f_{Ion}		f_{Ion}		f_{Ion}
1	MgO		InP		H-C	
2	SiC		GaAs		H-O	
3	BN		NaF		H-Cl	

2. Refractory metals (W, Ta, Nb, Mo, Re, Os, Ir) are characterized by extremely high melting points above 2000 °C. Can you suggest a possible reason for this?

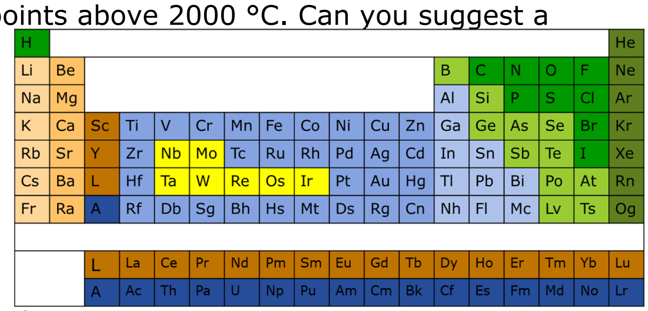


Group exercise

1. Find the fraction of ionic bonding for different chemical compounds and chemical bonds given by the number N of your breakout room.

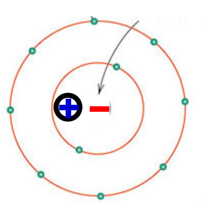
Group number N		f_{Ion}		f_{Ion}		f_{Ion}
1	MgO	73%	InP	4%	H-C	4%
2	SiC	12%	GaAs	4%	H-O	39%
3	BN	22%	NaF	91%	H-Cl	18%

2. Refractory metals (W, Ta, Nb, Mo, Re, Os, Ir) are characterized by extremely high melting points above 2000 °C. Can you suggest a possible reason for this?



Secondary bonds
Van der Waals bonding (London bonding)

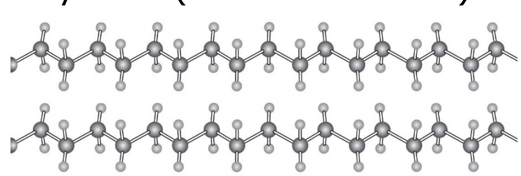
- Dipole-dipole interaction
- Permanent dipoles results from polar covalent bands
- Dipoles might be induced by collisions



- Weakest of all types of bonding

Examples

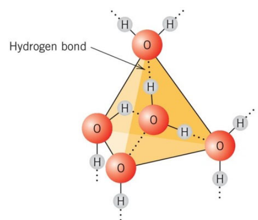
- Noble gases (He, Ar, …)
- Symmetrical molecules (CH_4, CCl_4, C_{60}, …)
- Molecules (NO, CO_2, …)
- Polymers (chain molecules)



Secondary bonds
Hydrogen bond

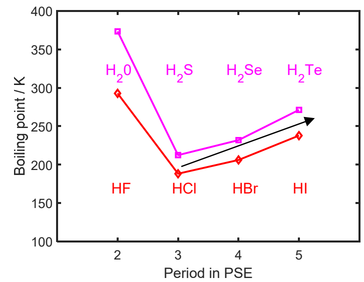
- Hydrogen ion = proton
- Hydrogen atom in covalent bond with electronegative atom

H-F···H-F



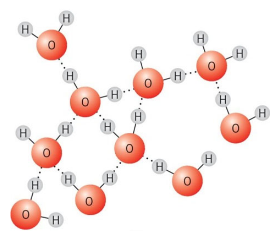
- Interaction with free electron pair (proton can switch between neighbors)

Examples
- H_2O, HF, …
- Biomolecules (Proteins, DNA)

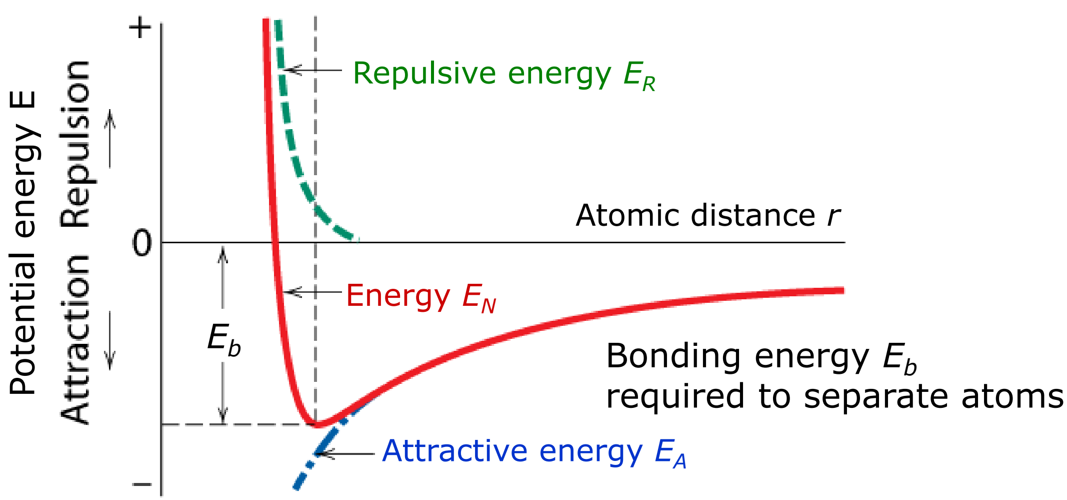


General: the higher the molar mass, the higher the melting temperature

Consequences
- High melting temperature
- High boiling temperature
- Low density as solid



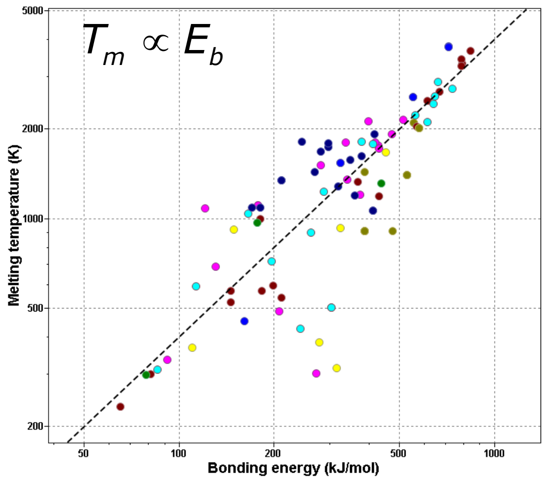
Bonding energy

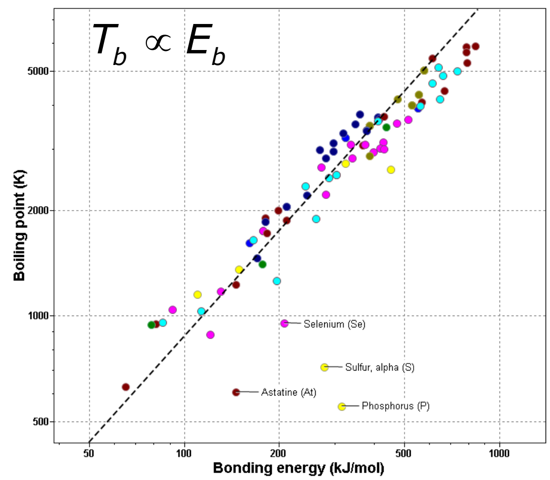


Affects materials properties
Bond energy → melting temperature (boiling temp.)
Energy profile → Elastic modulus, thermal expansion

Property correlations

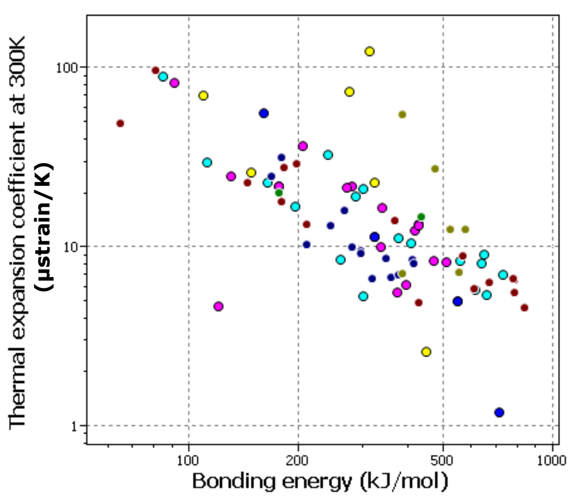
- Melting temperature T_m and bonding energy E_b
- Boiling temperature T_b and bonding energy E_b





Property correlations

- Thermal expansion coefficient and bonding energy E_b



Summary

Atomic bonds

Covalent bond	Ionic bond	Metallic bond

Secondary bonds

Material classes

Polymers	Ceramics	Metals

Consequences of atomic bonds

Melting temperature	Density	Resistivity

Bond types and material classes