Survey of semiconductor properties

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Survey of Semiconductor Properties

- Qualitative description of bond formation: arithmetics of covalent bond and tetrahedral coordination
- Relation between bandgap and lattice parameter in group IV semiconductors
- Orbital character of the valence band (VB) and conduction band (CB) in Si and Ge
- Ionic bonding in III-V and II-VI semiconductors
- Bandgap and lattice parameter in III-Vs and II-VIs
- Dichalcogenides
- Available substrates

Systematics of semiconductor bandgaps and crystal structure

	II	III	IV	V	VI
2	^{4}Be	^{5}B	^{6}C	^{7}N	^{8}O
3	^{12}Mg	^{13}Al	^{14}Si	^{15}P	^{16}S
4	^{30}Zn	^{31}Ga	^{32}Ge	^{33}As	^{34}Se
5	^{48}Cd	^{49}In	^{50}Sn	^{51}Sb	^{52}Te
6	^{80}Hg	^{81}Tl	^{82}Pb	^{83}Bi	^{84}Po
	S^2P^0	S^2P^1	S^2P^2	S^2P^3	S^2P^4

Semiconducting materials can be (mainly) obtained from:

- group IV elements
  - Si, Ge, SiC, SiGe, GeSn
- III-V alloys
  - binary: GaAs, GaP, InAs; ternary: $(In_xGa_{1-x})As$, $(In_xGa_{1-x})P$; quaternary: $(Al_xIn_yGa_{1-x-y})As$, $(In_xGa_{1-x})As_yP_{1-y}$
- II-VI alloys

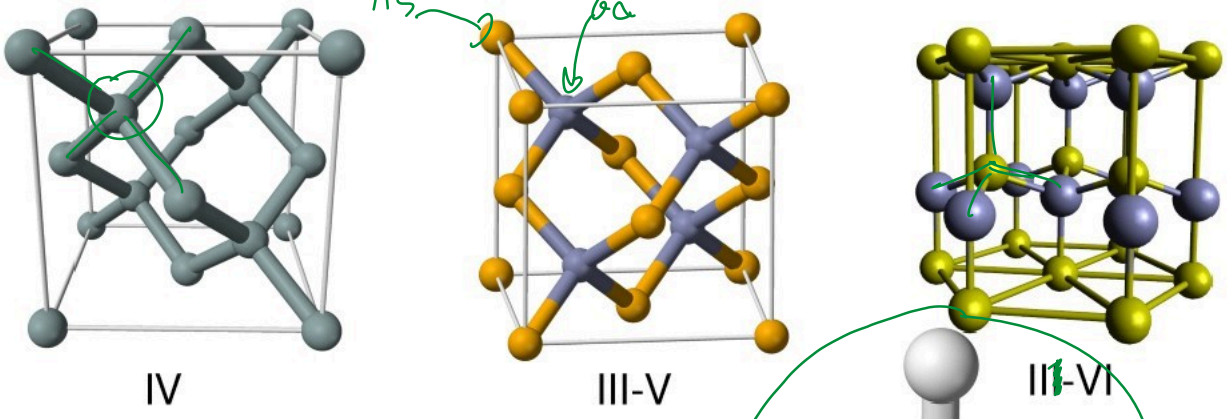
50% ⇒ 50%

- binary: CdTe, ZnTe; Ternary: $(Cd_xZn_{1-x})Te$, $(Hg_xCd_{1-x})Te$, $(Hg_xZn_{1-x})Se$

The arithmetic of semiconductors bonds

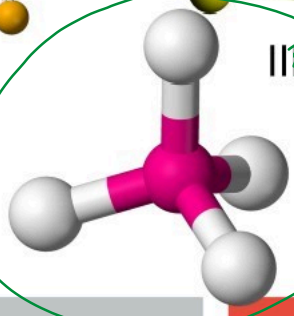
The average atomic configuration is $ns^2\,np^2$:
four electrons are required to complete the atomic shell $ns^2\,np^6$

Diamond (C) Zinc-blende (ZnSe) Wurtzite (ZnS)



IV III-V II-VI

The "lego block" of semiconductors crystals features a tetrahedral (**fourfold**) coordination



A semiconducting molecule

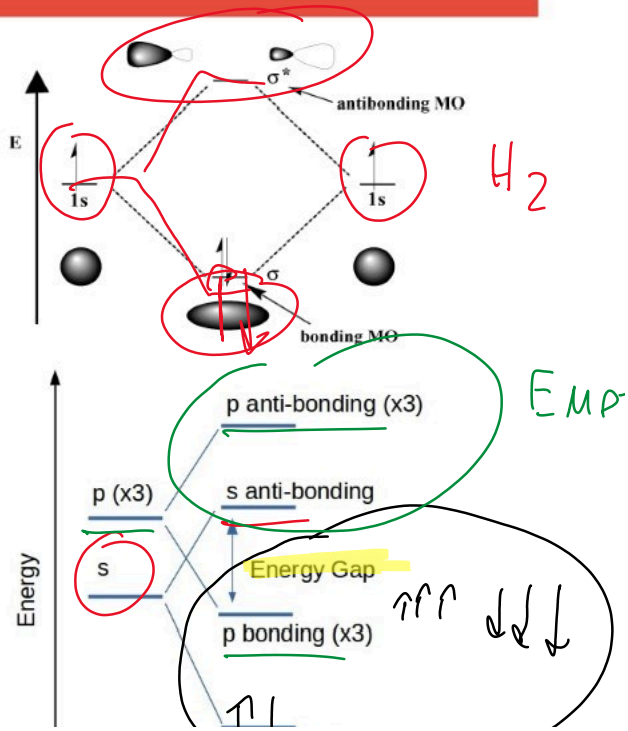
Hydrogen molecule
1 s orbitals form one bonding and one antibonding energy level.

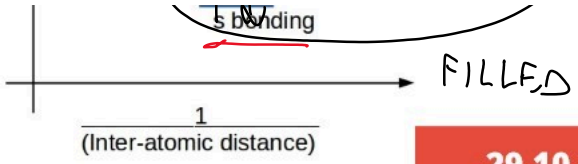
Semiconducting molecule
1 s orbitals + 3 p orbitals form:
1 + 3 = 4 bonding orbitals
1 + 3= 4 antibonding orbitals

The 4 bonding orbitals can host 8 electrons: 4 from the central atom + 4 from the near-neighbours

The bonding level is filled
The antibonding level is empty

We have a semiconductor!

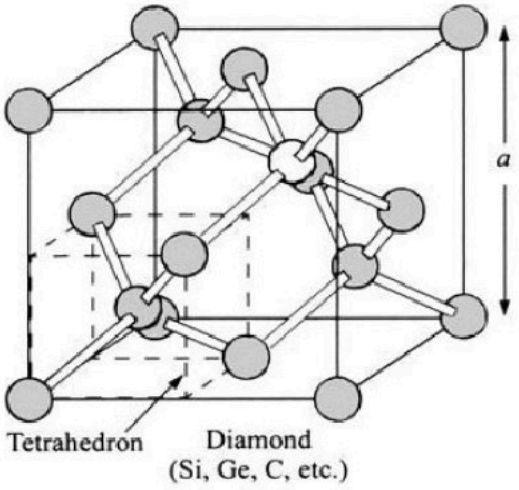




Lattice parameters and bandgaps in group IV SC

C, Si , Ge and α-Sn all crystallize in the

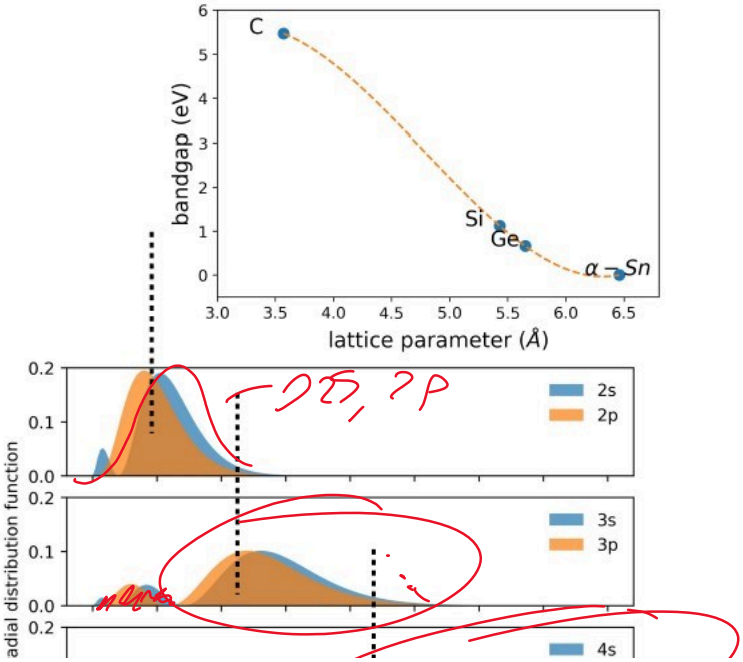
DIAMOND lattice
=
FCC with 2 atoms per lattice site
=
2 interpentrating FCC displaced by a/4<111>



	a (Å)	E_g (eV)	T (°C)
C	3.57	5.47	3547
Si	5.43	1.12	1412
Ge	5.65	0.66	937
α-Sn	6.46	-0.41	17

DIAMOND → β-Sn HEXAGONAL

Lattice parameters and bandgaps in Group IV SC



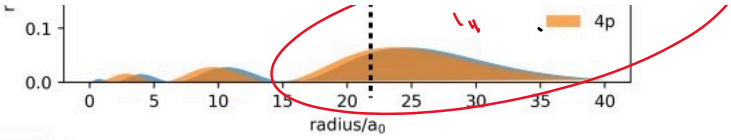
Smaller lattice parameter

↓

Larger bandgap

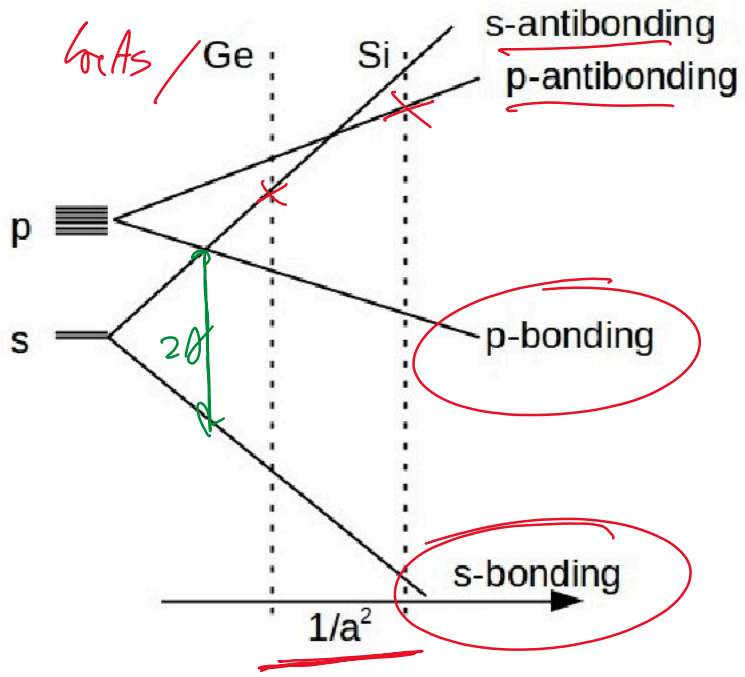
C-diamond

Si



Ge

Valence and Conduction band states in Si and Ge



The semiconducting molecule model gives

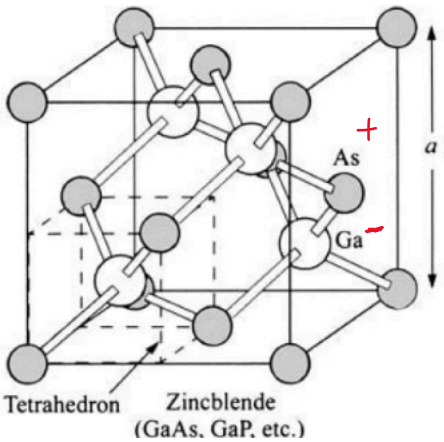
VB character: p-orbitals for Si and Ge

CB: p-orbitals for Si
s-orbital for Ge

Not completely (but almost) true

III-V and II-VI

Most III-V and II-VI semiconductors maintain a tetrahedral coordination between near-neighbours. The crystal structure is still FCC with a two atom basis. Since the two atoms are different the lattice is called zincblende like.



COVALENT + IONIC COMPOUND

The lattice is again given by two interpenetrating FCC lattices. Each lattice is occupied by a given atomic specie (i.e. Ga or As).

Ionic contribution to the atomic bond

3	Mg^{12}	Al^{13}	Si^{14}	P^{15}	S^{16}
4	Zn^{30}	Ga^{31}	Ge^{32}	As^{33}	Se^{34}
5	Cd^{48}	In^{49}	Sn^{50}	Sb^{51}	Te^{52}

	a (Å)	E_g (eV)
Ge	5.65	0.66
GaAs	5.65	1.52
ZnSe	5.67	2.83

Lattice parameters and bandgaps in III-V SC

Al^{13}	Si^{14}	P^{15}
Ga^{31}	Ge^{32}	As^{33}
In^{49}	Sn^{50}	Sb^{51}

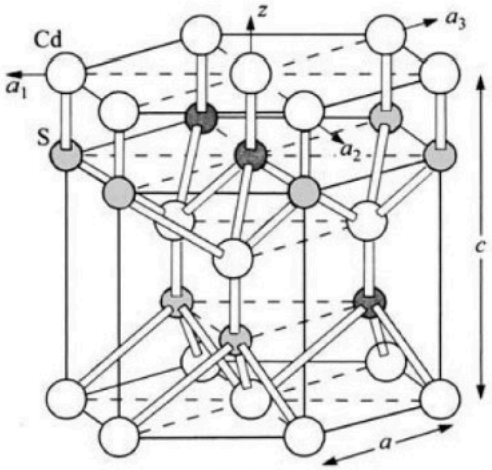
Al^{13}	Si^{14}	P^{15}
Ga^{31}	Ge^{32}	As^{33}
In^{49}	Sn^{50}	Sb^{51}

III\V	P	As	Sb
Al		2.16 eV/ 5.65 Å	
Ga	2.26 eV/5.45 Å	1.42 eV/5.65 Å	0.762 eV/ 6.09 Å

In	1.34 eV/5.86 Å	0.354 eV/6.06 Å	0.17 eV/6.48 Å

The Wurtzite crystal structure

When the bond has a high ionic component the crystal still maintains the tetrahedral coordination moving towards an hexagonal 'high packing' configuration.



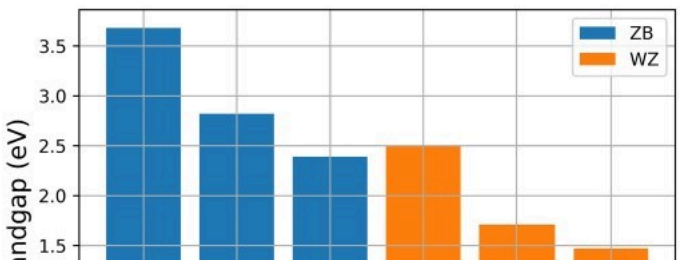
Wurtzite
(CdS, ZnS, etc.)

ZnSe (zincblende) and ZnS (wurtzite) crystallizes in both phases zincblende and wurtzite. GaN has a wurtzite lattice.

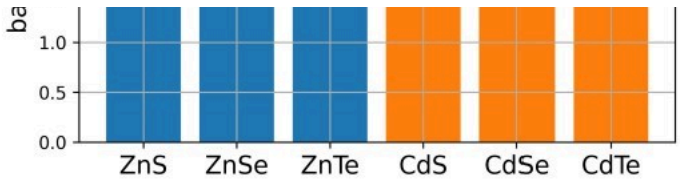
II-VI (monochalcogenides)

	II	III	IV	V	VI
2	^{4}Be	^{5}B	^{6}C	^{7}N	^{8}O
3	^{12}Mg	^{13}Al	^{14}Si	^{15}P	^{16}S
4	^{30}Zn	^{31}Ga	^{32}Ge	^{33}As	^{34}Se
5	^{48}Cd	^{49}In	^{50}Sn	^{51}Sb	^{52}Te
6	^{80}Hg	^{81}Tl	^{82}Pb	^{83}Bi	^{84}Po

chalcogens



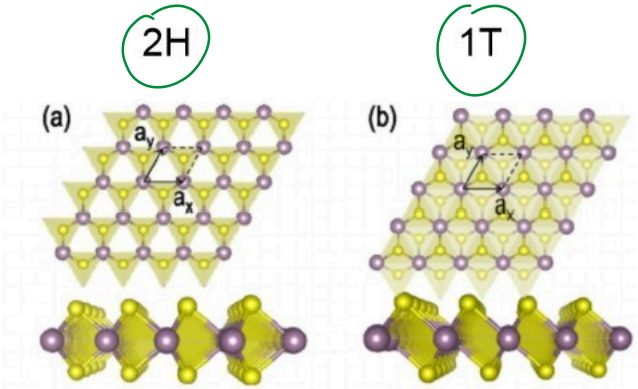
→ ZINC BLEN
→ WURTZITE

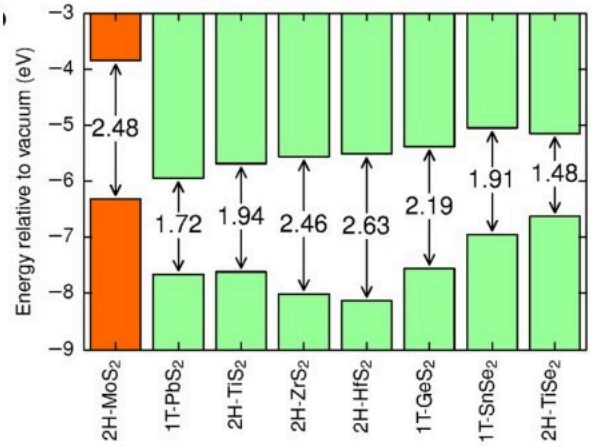


Transition Metal Dichalcogenides - TMDs

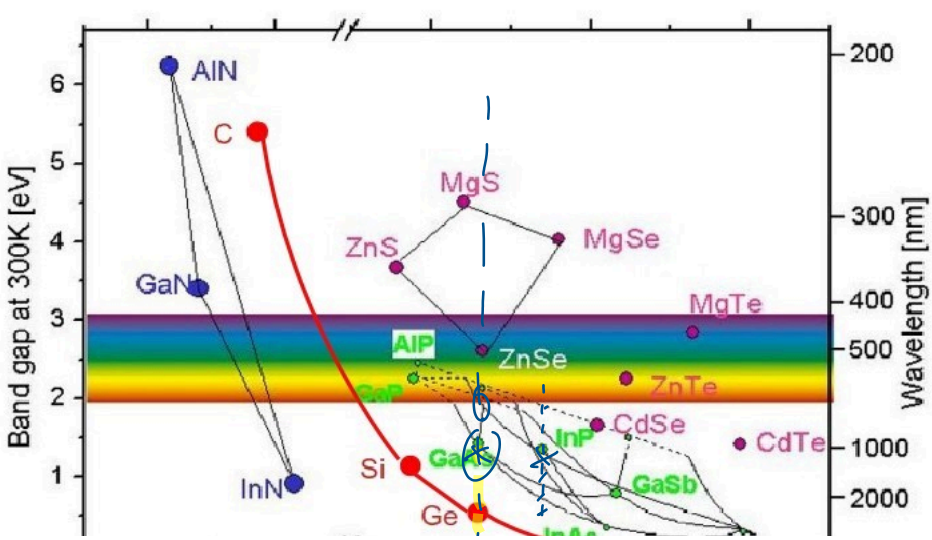
M=metal C=chalcogenides

Dichalcogenides MC_2: MoS_2, $TiSe_2$

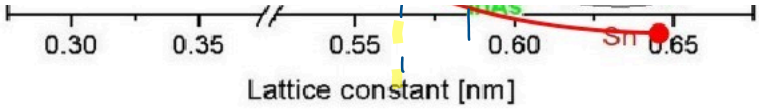




Lattice parameters and bandgaps



- IV
- III V
- II VI
- NITRIDES



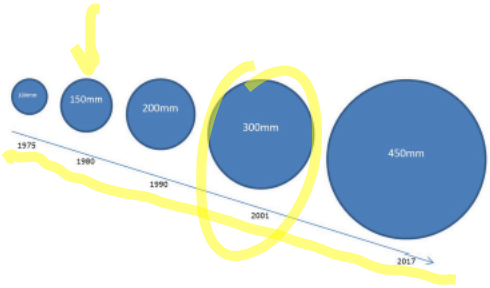
Substrates and epilayers

Si wafers: wafer size up to 300mm cost ≈ from 200 to 700 €

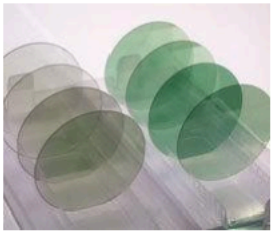
Ge wafers are used in high-efficiency multi-junction solar cells employed in space applications. Standard diameter 100 mm with cost ≈ 150 €

GaAs substrates are used for smartphone power amplifiers and switches, LEDs and solar cells.

InP substrates are used for optical communication modules. The max wafer size is 200 mm. Typical costs are a factor of 5 to 10 times higher than those a Si wafer.



SiC: is a key material for power electronics thanks to its large bangap and high thermal conductivity. Wafers can be purchased in diameters up to 150 mm at a price of ≈ 500 € .



Sapphire: Al_2O_3 is an insulator, it is used as a substrate for the deposition of GaN, a key material for LED and high power electronics. A 100 mm wafer costs approximately 20 €.