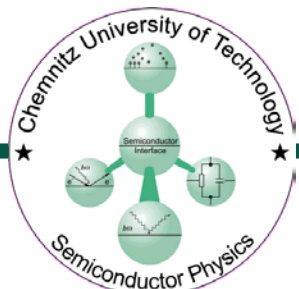


General Properties of Semiconductors





Topics

General Properties of Semiconductors

Crystal Structure

(Feiertag)

The Reciprocal Space & The Fourier Transform

X-Ray Diffraction basics & Multipurpose X-Ray Diffraction systems with built-in intelligent guidance.

Lattice Vibrations & Phonons / Dispersion Relations & Density of States (DOS)

Phonon Spectroscopies: Raman & Infra Red

Atomic Structure & Chemical Bonding

Electronic properties of Semiconductors (intro.)

Electronic properties of Semiconductors (cont.)

(Feiertag)

Electronic properties of Semiconductors (end)

(Feiertag)

Spectroscopic methods for electronic and optical properties characterization

The Nano-World! (intro): From Micro to Nanospectroscopy/ from Micro to Nanomaterials

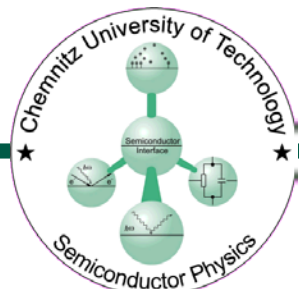
Solid Surfaces & Interfaces

Heterojunctions, Heterostructures and Quantum Confined Structures

Techniques for Synthesis of Nanomaterials

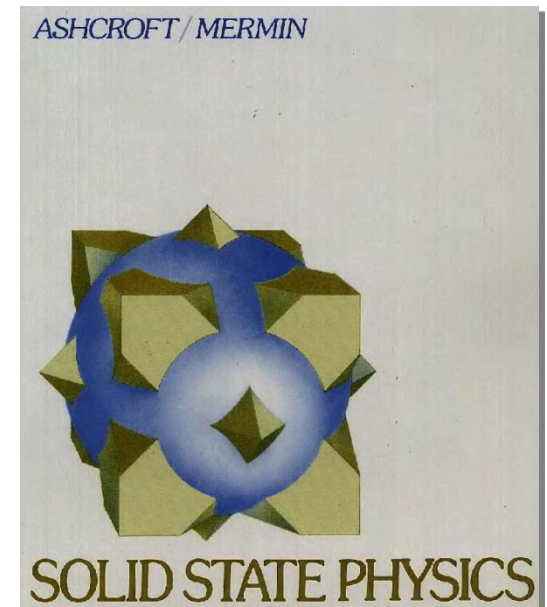
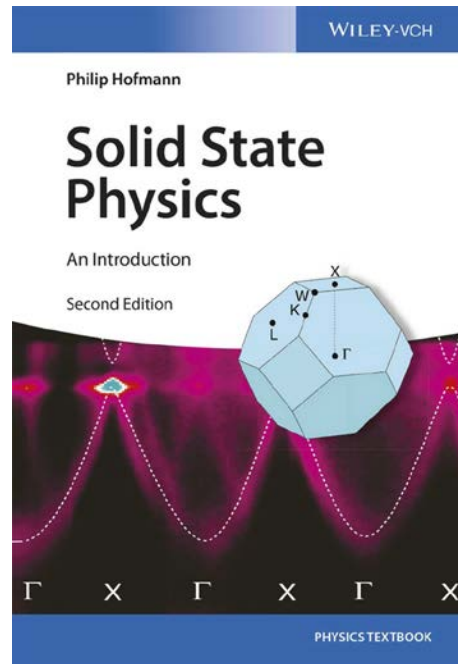
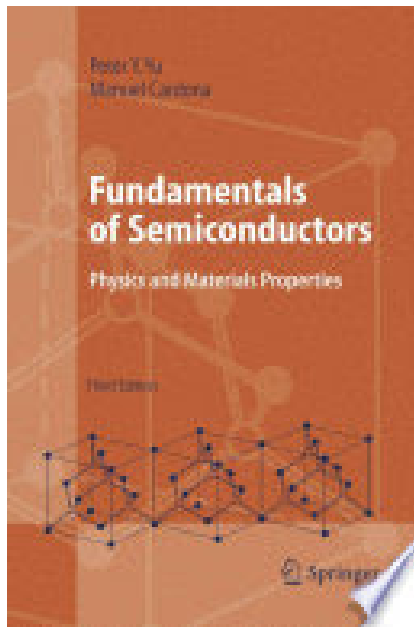
Understanding (the relevance of) Quantum Mechanics - a light introduction

Dedicated sessions for revisions (lectures & exercises)



Recommended Literature

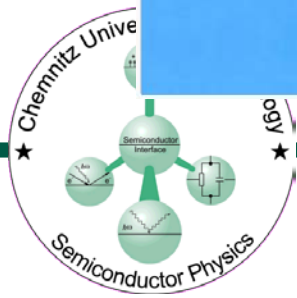
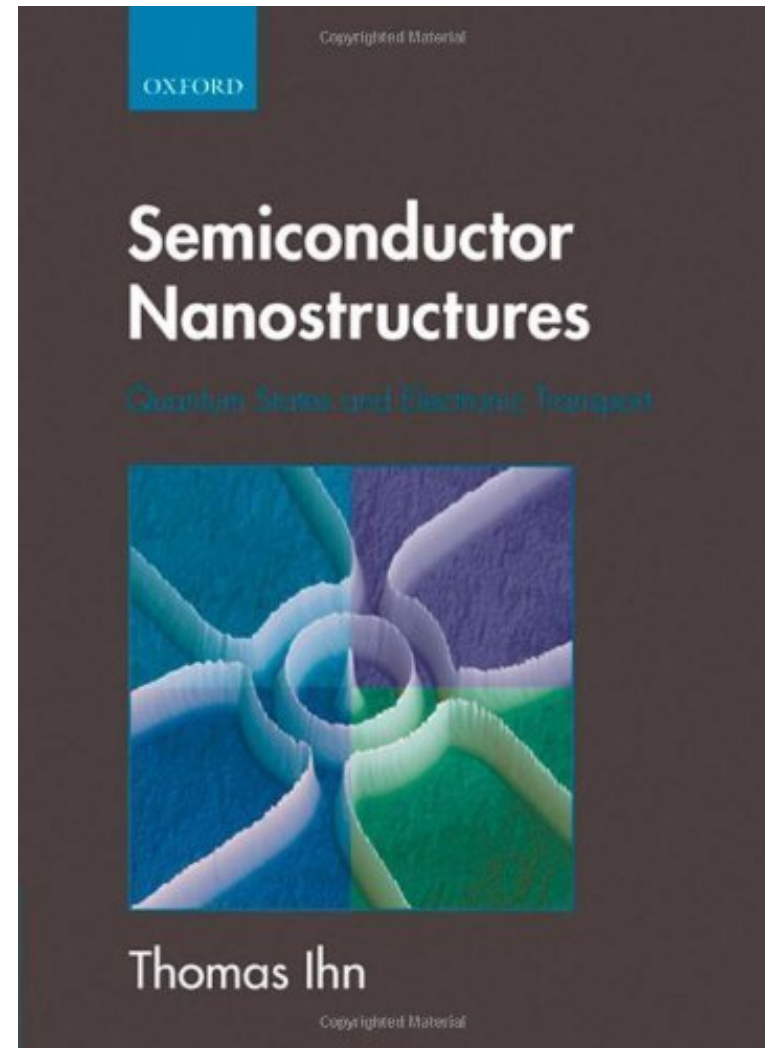
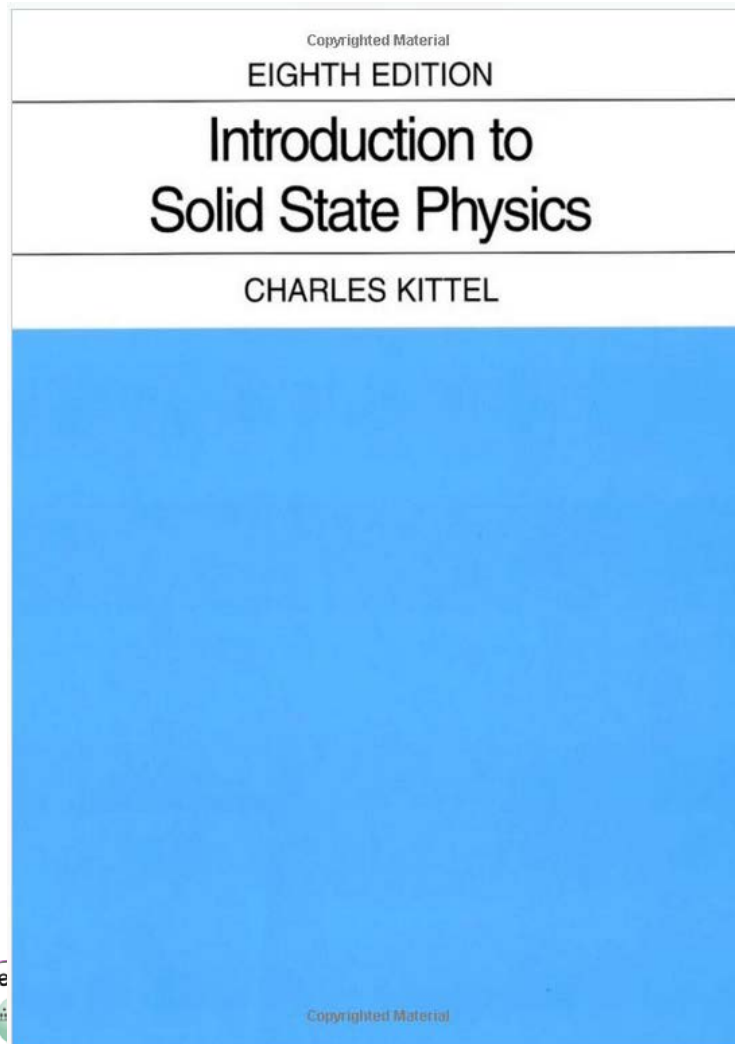
E- Books available via TUC library!



<https://katalog.bibliothek.tu-chemnitz.de/Record/0007291792>

<http://lib.mylibrary.com/Open.aspx?id=788237>





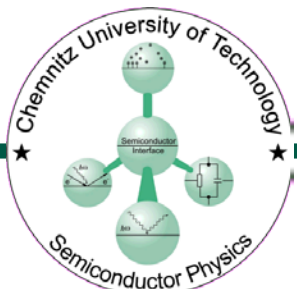
THE HISTORY OF SEMICONDUCTORS

? HOW OLD IS SEMICONDUCTOR SCIENCE ?

Not clear!

First experiments performed 200 years ago!

The concept of 'semiconductor' appears in early 20th century.



History of Semiconductors

https://djena.engineering.cornell.edu/hws/history_of_semiconductors.pdf

1782 Alessandro Volta: “semiconducting” term is used for the first time.

1821 Humphry Devy: discovers the increase in resistivity of metals with increasing temperature.

1833 Michael Faraday: observed the first exception to Devy’s experimental results: the decrease of resistivity to metallic values with increase of temperature of Silver Sulfide (Ag_2S).

1874 Karl Braun: discovers and documents the first semiconductor diode effect; he observed that current flows freely in only one direction at the contact between a metal point and a galena crystal.

1901 Jagadis Chandra Bose: invents and patents the very first semiconductor device called “cat whiskers”. Cat whiskers was a point-contact semiconductor rectifier used for detecting radio waves.

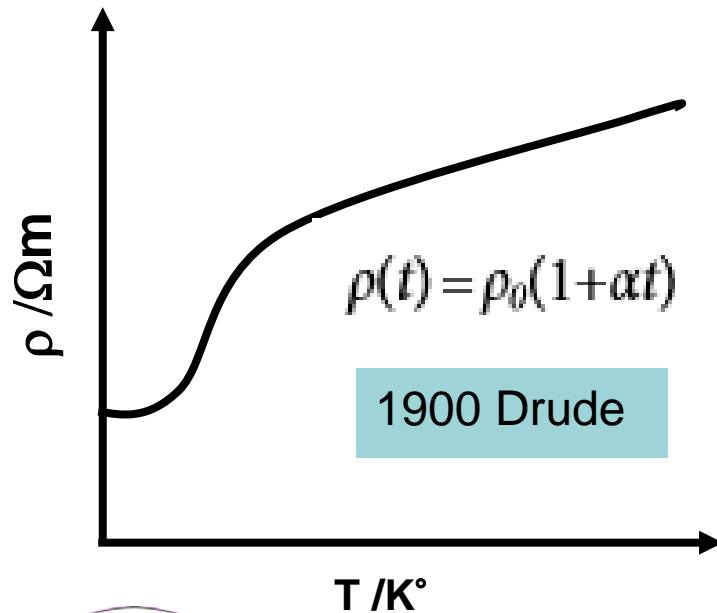
1901 Drude provides the first mathematical expression for the phenomena observed by H. Devy.

1908 Johann Koenigsberger and Schilling provide the first mathematical expression for the phenomena observed by of M. Faraday.

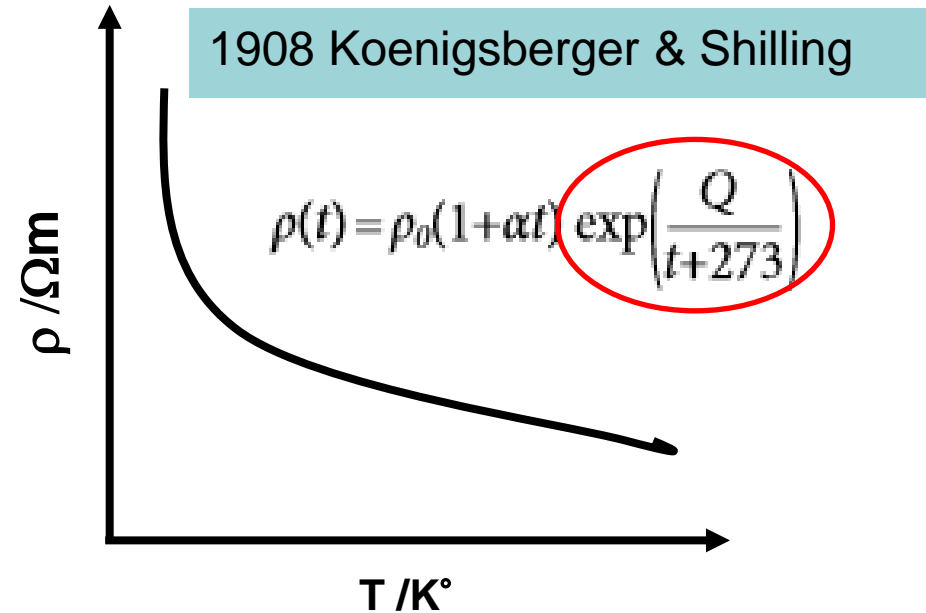
One of the first properties observed that distinguished semiconductors from conductors was the

Variation of resistivity (ρ) with temperature (T)

Conductor



Semiconductor



Koenigsberger could not propose any physical model for the origin of the dissociation Energy – Q – but based on this he divides all materials into:

metals insulators “variable conductors”

- ✓ for insulators Q is infinitely large (so there are no free electrons);
- ✓ for metals at high temperatures $Q=0$ (i.e. nr of electrons in metals is equal to the number of ions (= basic assumption of Drude’s theory);
- ✓ for “variable conductors” Q is finite; therefore their resistivity decreases exponentially with increasing temperature;
- ✓ demonstrates experimentally that Q depends critically on the material purity and the presence of defects.

1931 Alan Wilson Proposes **Band Theory of Semiconductors** after quantum mechanics is established; draws the picture of energy bands and energy gaps in between, giving like this physical meaning to the Koenigsberger's dissociation energy.

1931 Werner Heisenberg Concept of “holes” - carriers with positive charge, presenting unoccupied positions in the mainly occupied valence band.

Birth of Semiconductor Science



1914



Koenigsberger

WHY ?!

Since that time it was possible to speak about a new class of solids with strictly defined properties, rather than separate “anomalous” materials.

Although the basic features of semiconductor theory were developed in the 1930s, semiconductors remained “unpopular” until the mid 1940s for lack of suitable technologies.

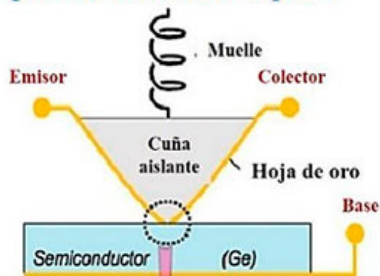
All crystals were “dirty”, and results obtained were irreproducible!

William Shockley, John Bardeen and **Walter Brattain**,
discover transistor action in germanium in 1947

1951

changed the situation after the fabrication of the first transistor on p-n junctions.

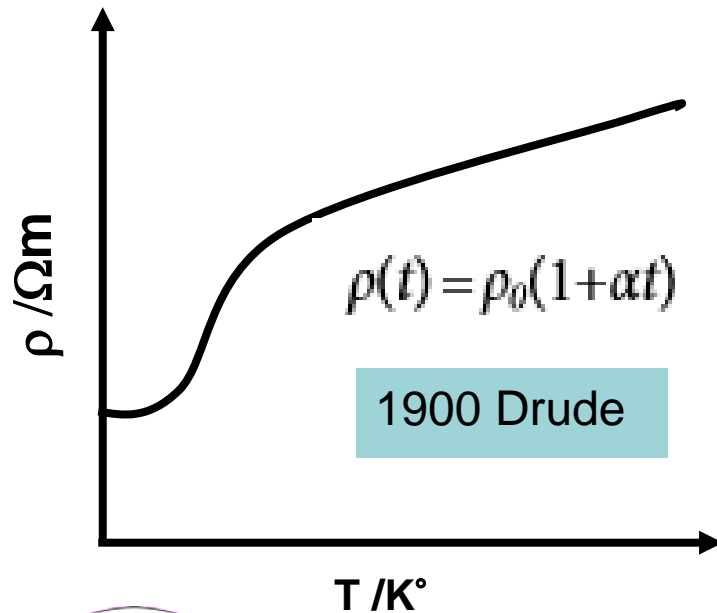
Esquema del
primer transistor bipolar



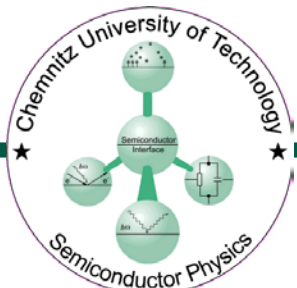
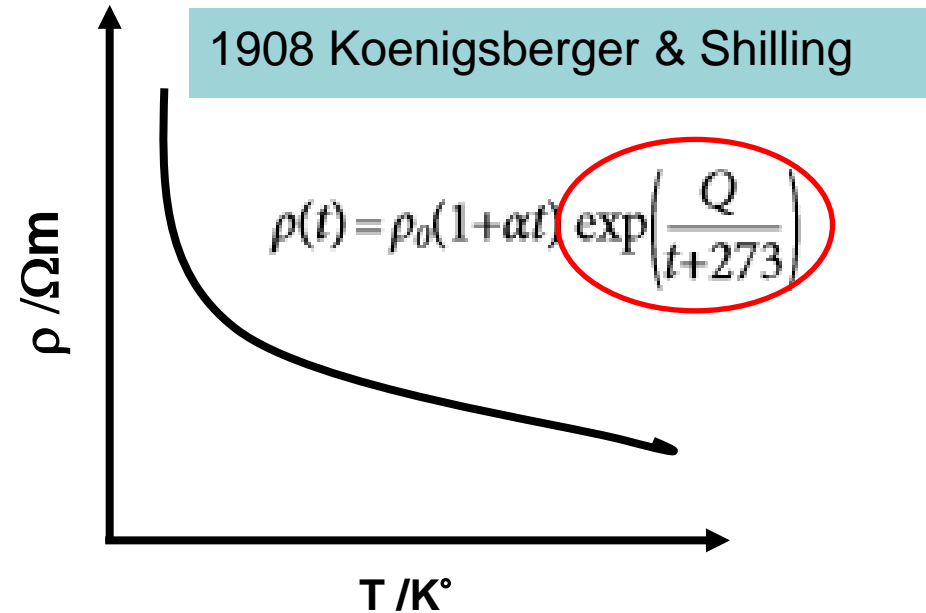


Resistivity (ρ) decreases with increasing temperature (T)

Conductor



Semiconductor



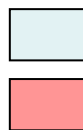
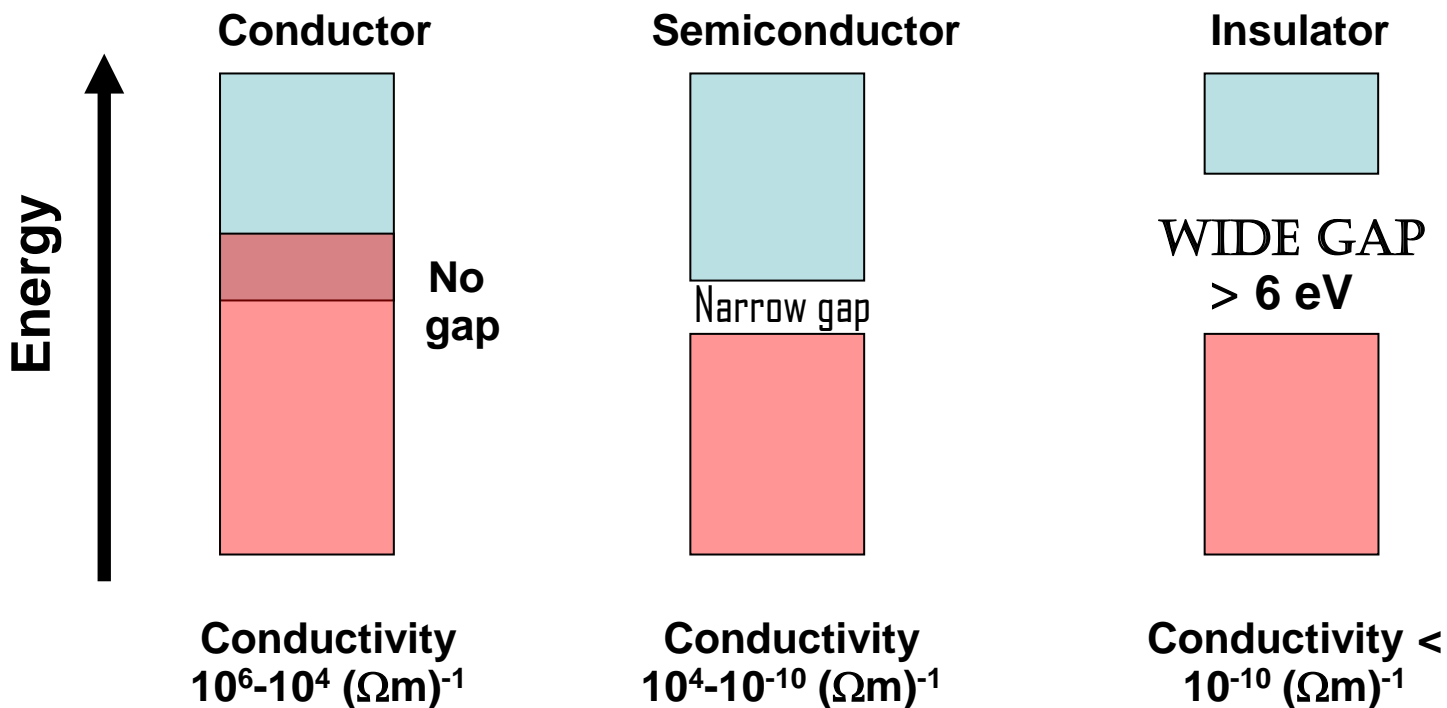


1. General Properties of Semiconductors

1st Lecture

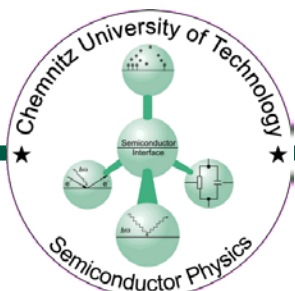
1.1. Qualitative Properties

! Band Gap < 6 eV !



Conduction Band (CB)

Valence Band (CB)





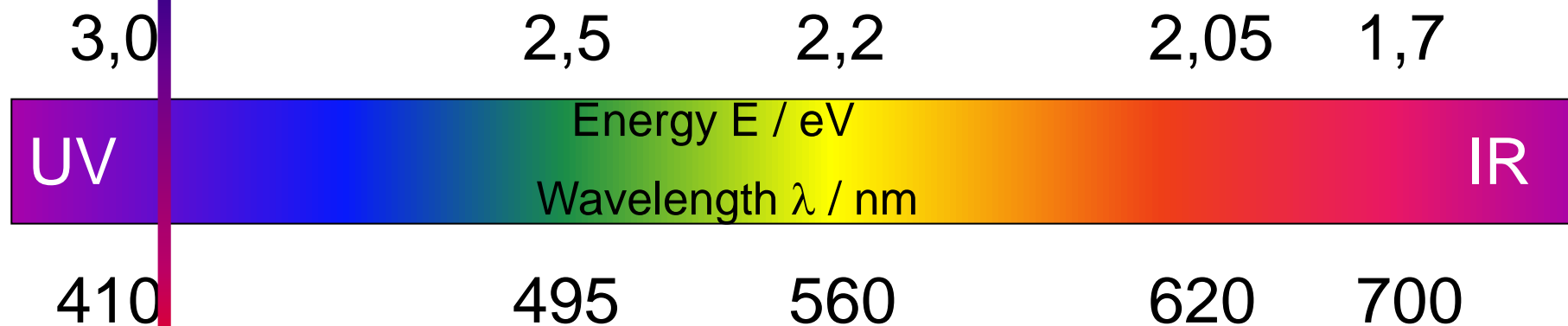
1. General Properties of Semiconductors

1st Lecture

1.1. Qualitative Properties

Typical

energy range [eV] and absorption wavelengths [nm] of band gaps.



! More info in the **Semiconductor Master Graph** !

$$E[\text{eV}] = \frac{1240}{\text{photon wavelength [nm]}}$$

$$1 \text{ eV} = 1,602 \times 10^{-19} \text{ J}$$

25 meV: thermal energy $k_B T$ at room temperature (300 K)

$$1 \text{ nm} = 10^{-9} \text{ m} = 10 \text{ \AA}$$

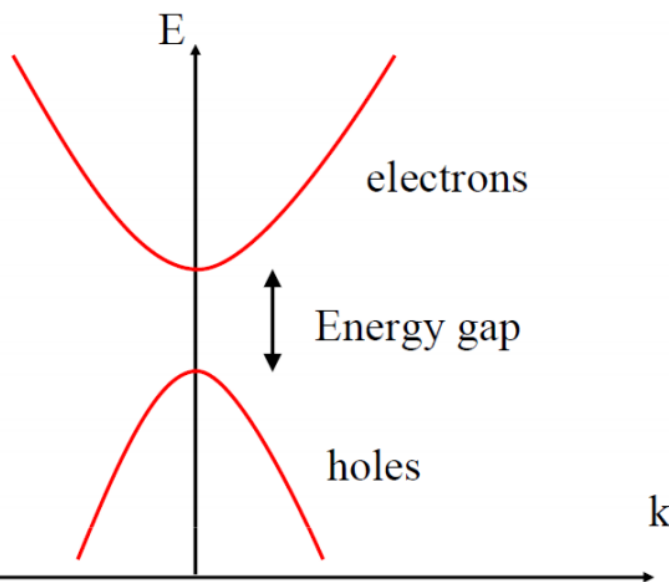


The band gap of a semiconductor is always one of two types:

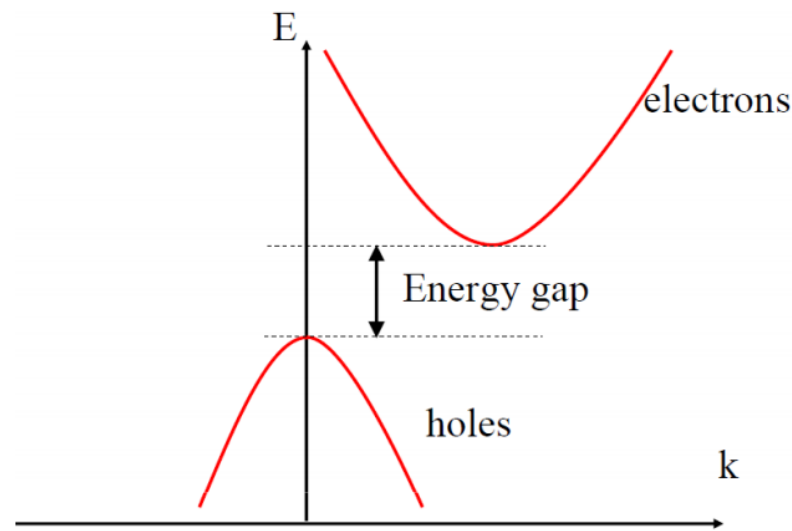
direct band gap

or

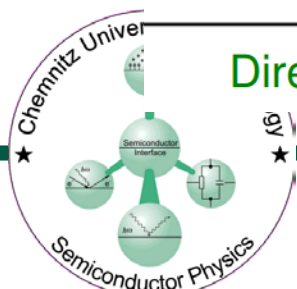
indirect band gap



Direct bandgap semiconductors



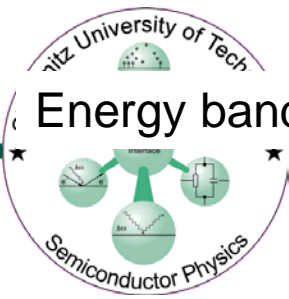
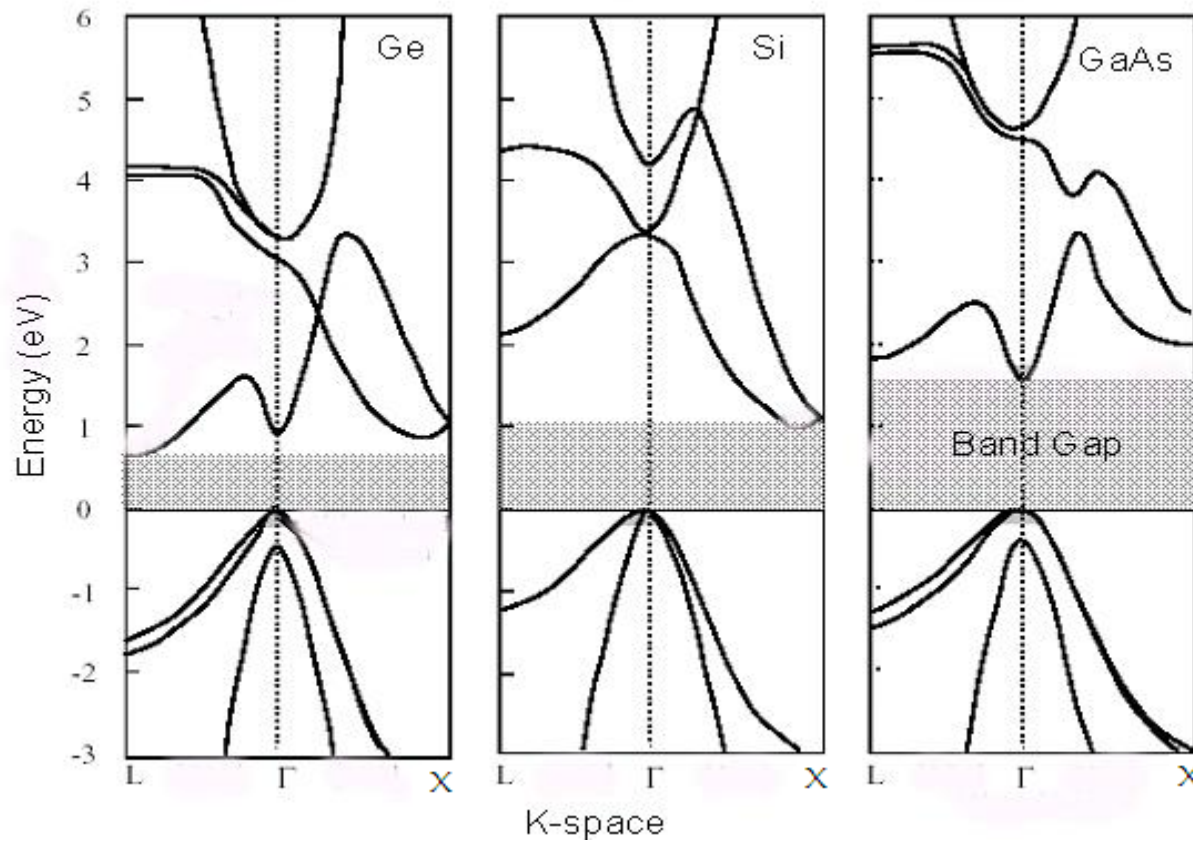
Indirect bandgap semiconductors





In real life band gaps don't look like this are more complex due to semiconductors

Crystal Structure and atomic size



Energy band diagram of Germanium (Ge), Silicon (Si) and Gallium Arsenide (GaAs)



1. General Properties of Semiconductors

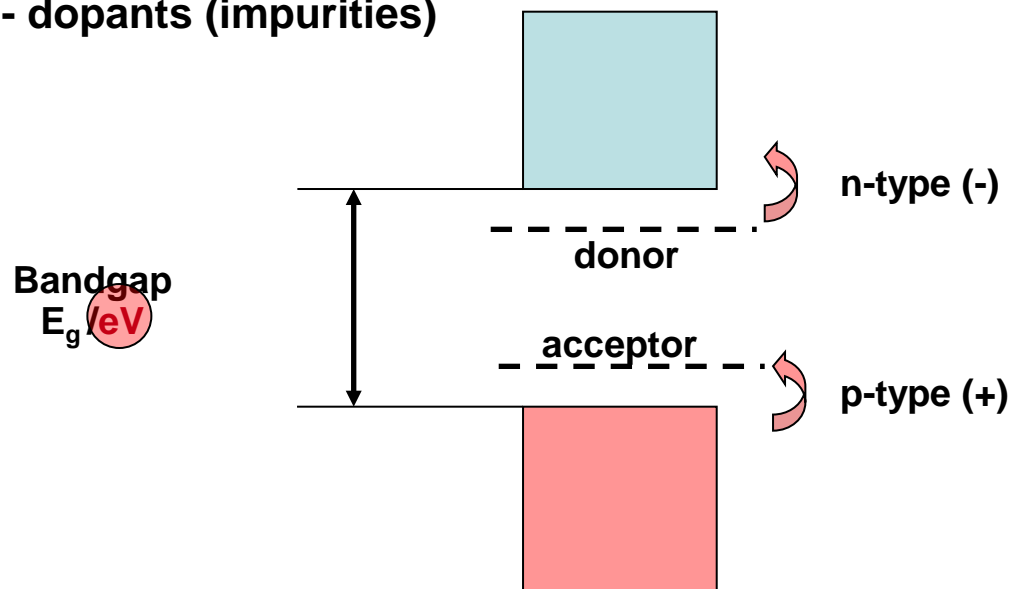
1st Lecture

1.1. Qualitative Properties

Intrinsic semiconductors

Extrinsic semiconductor

- dopants (impurities)



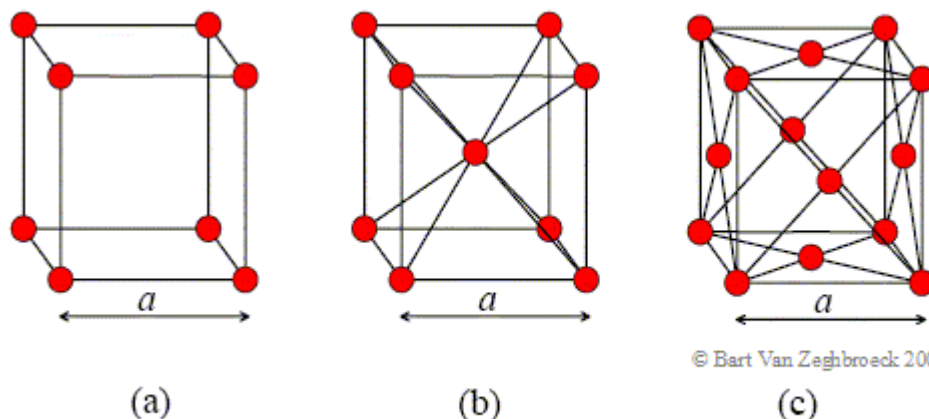
Which goes back to Koenigsburg observation:

Semiconductors properties vary with impurity and defects!



Semiconductors are also as a **crystalline material**, consisting of atoms arranged in a highly ordered pattern, called ***lattice*** (we shall discuss this little later).

Typical Semiconductor
Crystal Structures!



The simple cubic (a), the body-centered cubic (b) and the face centered cubic (c) lattice.

Though all materials may not be necessarily crystalline (could be either quasi crystalline or amorphous), but in the short-range or at the microscopic level, they are crystalline.

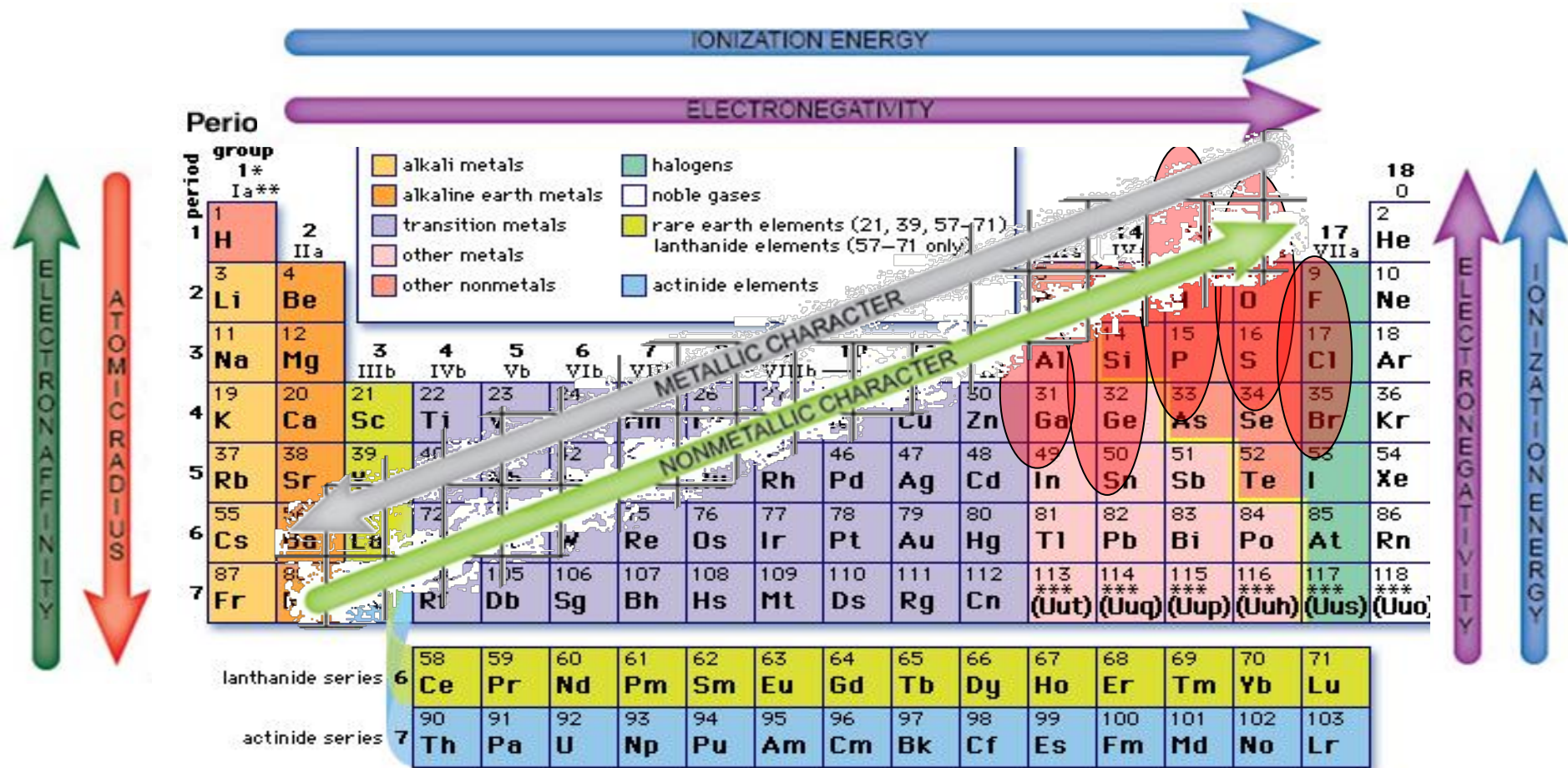
Once we treat the lattice as a periodic potential, we see remarkable properties that explain the physical nature of semiconductors.



1. General Properties of Semiconductors

1st Lecture

1.1. Qualitative Properties

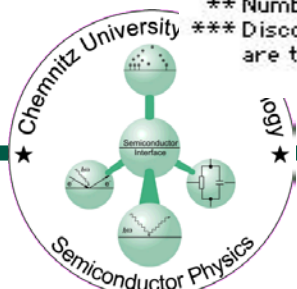


* Numbering system adopted by the International Union of Pure and Applied Chemistry (IUPAC).

** Numbering system widely used, especially in the U.S., from the mid-20th century.

*** Discoveries of elements 113-118 are claimed but not confirmed. Element names and symbols in parentheses are temporarily assigned by IUPAC.

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12.04.2021



IMPORTANT NOTICE! New IUPAC names:

1st Lecture

IUPAC INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY



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DATABASES

PERIODIC TABLE OF ELEMENTS

CONFERENCES

AWARDS

PERIODIC TABLE OF ELEMENTS

1

H

hydrogen

[1.0078, 1.0082]

2

3

Li

lithium

[6.938, 6.997]

4

5

Be

beryllium

9.0122

6

7

B

boron

[10.806, 10.821]

8

9

C

carbon

[12.009, 12.012]

9

10

N

nitrogen

[14.006, 14.008]

10

11

O

oxygen

[15.999, 16.003]

11

12

F

fluorine

18.998

12

13

Ne

neon

20.180

13

Na

sodium

[22.990, 22.990]

14

15

Mg

magnesium

[24.304, 24.307]

15

16

Al

aluminum

[26.981, 26.982]

16

17

Si

silicon

[28.085, 28.086]

17

18

P

phosphorus

[30.973, 30.974]

18

19

S

sulfur

[32.059, 32.077]

19

20

Cl

chlorine

[35.45, 35.457]

20

21

Ar

argon

39.962

21

K

potassium

[39.098, 39.098]

22

23

Ca

calcium

[40.078(4), 40.078]

23

24

Sc

scandium

44.956

24

25

Ti

titanium

47.867

25

26

V

vanadium

50.942

26

27

Cr

chromium

51.996

27

28

Mn

manganese

54.938

28

29

Fe

iron

[55.845(2), 55.845]

29

30

Co

cobalt

58.933

30

31

Ni

nickel

[58.693, 58.693]

31

32

Cu

copper

[63.546(3), 63.546]

32

33

Zn

zinc

[65.38(2), 65.382]

33

34

Ga

gallium

[69.723, 69.723]

34

35

Ge

germanium

[72.630(8), 72.630]

35

36

As

arsenic

[74.922, 74.922]

36

37

Se

selenium

[78.971(8), 78.971]

37

38

Br

bromine

[79.904, 79.904]

38

39

Kr

krypton

[83.798(2), 83.798]

39

Rb

rubidium

[85.468, 85.468]

40

41

Sr

strontium

[87.62, 87.62]

41

42

Y

yttrium

88.906

42

43

Zr

zirconium

[91.224(2), 91.224]

43

44

Nb

niobium

92.906

44

45

Mo

molybdenum

95.95

45

46

Tc

technetium

[98.01(2), 98.01]

46

47

Ru

ruthenium

[101.07(2), 101.07]

47

48

Rh

rhodium

102.91

48

49

Pd

palladium

106.42

49

50

Ag

silver

107.87

50

51

Cd

cadmium

112.41

51

52

In

indium

114.82

52

53

Sn

tin

118.71

53

54

Sb

antimony

121.76

54

55

Te

tellurium

[127.60(3), 127.60]

55

56

I

iodine

126.90

56

57

Xe

xenon

[131.29, 131.29]

57

Cs

caesium

[132.91, 132.91]

58

59

Ba

barium

[137.33, 137.33]

59

60

La

lanthanide

89-103

60

61

Ce

cerium

138.91

61

62

Pr

praseodymium

140.91

62

63

Nd

neodymium

144.24

63

64

Pm

promethium

[144.91, 144.91]

64

65

Sm

samarium

[150.36(2), 150.36]

65

66

Eu

europium

151.96

66

67

Gd

gadolinium

157.25

67

68

Tb

terbium

158.93

68

69

Dy

dysprosium

162.50

69

70

Ho

holmium

164.93

70

71

Er

erbium

167.26

71

72

Tm

thulium

168.93

72

73

Yb

ytterbium

173.05

73

74

Lu

lutetium

174.97

74

Fr

francium

87

75

76

Ra

radium

88

76

77

Ac

actinide

89-103

77

78

Th

thorium

232.04

78

79

Pa

protactinium

231.04

79

80

U

uranium

238.03

80

81

Np

neptunium

[237.04, 237.04]

81

82

Pu

plutonium

[244.06, 244.06]

82

83

Am

americium

[243.06, 243.06]

83

84

Cm

curium

[247.07, 247.07]

84

85

Bk

berkelium

[247.07, 247.07]

85

86

Cf

californium

[251.08, 251.08]

86

87

Es

einsteinium

[252.08, 252.08]

87

88

Fm

fermium

[257.10, 257.10]

88

89

Md

mendelevium

[258.10, 258.10]

89

90

No

nobelium

[259.10, 259.10]

90

91

Lr

lawrencium

[262.10, 262.10]

91

La

lanthanum

138.91

92

93

Ce

cerium

140.12

93

94

Pr

praseodymium

140.91

94

95

Nd

neodymium

144.24

95

96

Pm

promethium

[144.91, 144.91]

96

97

Sm

samarium

[150.36(2), 150.36]

97

98

Eu

europium

151.96

98

99

Gd

gadolinium

157.25

99

100

Tb

terbium

158.93

100

101

Dy

dysprosium

162.50

101

102

Ho

holmium

164.93

102

103

Er

erbium

167.26

103

104

Tm

thulium

168.93

104

105

Yb

ytterbium

173.05

105

106

Lu

lutetium

174.97

106

Fr

francium

87

107

108

Ra

radium

88

108

109

Ac

actinide

89-103

109

110

Th

thorium

232.04

110

111

Pa

protactinium

231.04

111

112

U

uranium

238.03

112

113

Np

neptunium

[237.04, 237.04]

113

114

Pu

plutonium

[244.06, 244.06]

114

115

Am

americium

[243.06, 243.06]

115

116

Cm

curium

[247.07, 247.07]

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117

Bk

berkelium

[247.07, 247.07]

117

118

Cf

californium

[251.08, 251.08]

118

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Es

einsteinium

[252.08, 252.08]

119

120

Fm

fermium

[257.10, 257.10]

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121

Md

mendelevium

[258.10, 258.10]

121

122

No

nobelium

[259.10, 259.10]

122

123

Lr

lawrencium

[262.10, 262.10]

1

H

hydrogen

[1.0078, 1.0082]

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Li

lithium

[6.938, 6.997]

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Be

beryllium

9.0122

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[15.999, 16.003]

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54.938

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[58.693, 58.693]

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zinc

[65.38(2), 65.382]

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[69.723, 69.723]

34

35

Ge

germanium

[72.630(8), 72.630]

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36

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[74.922, 74.922]

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selenium

[78.971(8), 78.971]

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strontium

[87.62, 87.62]

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Y

yttrium

88.906

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44

Nb

niobium

92.906

44

45

Mo

molybdenum

95.95

45

46

Tc

technetium

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47

Ru

ruthenium

[101.07(2), 101.07]

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48

Rh

rhodium

102.91

48

49

Pd

palladium

106.42

49

50

Ag

silver

107.87

50

51

Cd

cadmium

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51

52

In

indium

114.82

52

53

Sn

tin

118.71

53

54

Sb

antimony

121.76

54

55

Te

tellurium

[127.60(3), 127.60]

55

56

I

iodine

126.90

56

57

Xe

xenon

[131.29, 131.29]

57

Cs

caesium

[132.91, 132.91]

58

59

Ba

barium

[137.33, 137.33]

59

60

La

lanthanide

89-103

60

61

Ce

cerium

138.91

61

62

Pr

praseodymium

140.91

62

63

Nd

neodymium

144.24

63

64

Pm

promethium

[144.91, 144.91]

64

65

Sm

samarium

[150.36(2), 150.36]

65

66

Eu

europium

151.96

66

67

Gd

gadolinium

157.25

67

68

Tb

terbium

158.93

68

69

Dy

dysprosium

162.50

69

70

Ho

holmium

164.93

70

71

Er

erbium

167.26

71

72

Tm

thulium

168.93

72

73

Yb

ytterbium

173.05

73

74

Lu

lutetium

174.97

74

Fr

francium

87

75

76

Ra

radium

88

76

77

Ac

actinide

89-103

77

78

Th

thorium

232.04

78

79

Pa

protactinium

231.04

79

80

U

uranium

238.03

80

81

Np

neptunium

[237.04, 237.04]

81

82

Pu

plutonium

[244.06, 244.06]

82

83

Am

americium

[243.06, 243.06]

83

84

Cm

curium

[247.07, 247.07]

84

85

Bk

berkelium

[247.07, 247.07]

85

86

Cf

californium

[251.08, 251.08]

86

87

Es

einsteinium

[252.08, 252.08]

87

88

Fm

fermium

[257.10, 257.10]

88

89

Md

mendelevium

[258.10, 258.10]

89

90

No

nobelium

[259.10, 259.10]

90

91

Lr

lawrencium

[262.10, 262.10]

1

H

hydrogen

[1.0078, 1.0082]

2

3

Li

lithium

[6.938, 6.997]

4

5

Be

beryllium

9.0122

6

7

B

boron

[10.806, 10.821]

8

9

C

carbon

[12.009, 12.012]

9

10

N

nitrogen

[14.006, 14.008]

10

11

O

oxygen

[15.999, 16.003]

11

12

F

fluorine

18.998

12

13

Ne

neon

20.180

13

Na

sodium

[22.990, 22.990]

14

15

Mg

magnesium

[24.304, 24.307]

15

16

Al

aluminum

[26.981, 26.982]

16

17

Si

silicon

[28.085, 28.086]

17

18

P

phosphorus

[30.973, 30.974]

18

19

S

sulfur

[32.059, 32.077]

19

20

Cl

chlorine

[35.45, 35.457]

20

21

Ar

argon

39.962

21

K

potassium

[39.098, 39.098]

22

23

Ca

calcium

[40.078(4), 40.078]

23

24

Sc

scandium

44.956

24

25

Ti

titanium

47.867

25

26

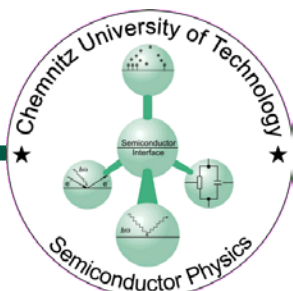
V



For notes and updates to this table, see www.iupac.org. This version is dated 1 December 2018.
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https://iupac.org/wp-content/uploads/2018/12/IUPAC_Periodic_Table-01Dec18.jpg



<https://iupac.org/what-we-do/periodic-table-of-elements/>

Semiconductor Physics / Micro and Nano

12.04.2021



1. General Properties of Semiconductors

1st Lecture

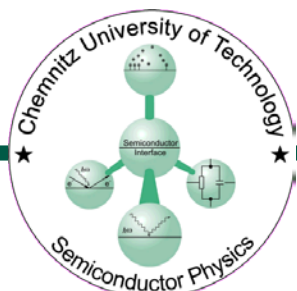
1.1. Qualitative Properties

Old IUPAC notation **BUT** Semiconductors classified accordingly!

Elemental Semiconductors

Type	Elements	Bandgap (E_g) /eV
IV	C	5.3
IV	Si	1.1
IV	Ge	0.7
IV	SiC (binary compound)	2.8

		IIIA	IVA	VA	VIA	VIIA	0
		5	6	7	8	9	10
		B	C	N	O	F	Ne
		13	14	15	16	17	18
		Al	Si	P	S	Cl	Ar
B	IB	31	32	33	34	35	36
Cu	Zn	Ga	Ge	As	Se	Br	Kr
Ag	Cd	In	Sn	Sb	Te	I	Xe
Au	Hg	Tl	Pb	Bi	Po	At	Rn





1. General Properties of Semiconductors

1st Lecture

1.1. Qualitative Properties

Binary Compounds (covalent bonding)

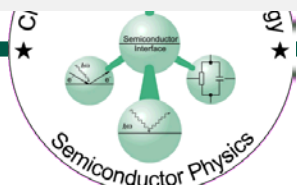
Type	Elements	Bandgap (E_g) /eV
III-V	BN	5.2
III-V	AlN	6.3
III-V	GaN	3.4
	InN	0.7



		IIIA	IVA	VA	VIA	VIIA	0
		5	6	7	8	9	10
		B	C	N	O	F	Ne
		13	14	15	16	17	18
		Al	Si	P	S	Cl	Ar
B	IB	31	32	33	34	35	36
Cu	Zn	Ga	Ge	As	Se	Br	Kr
Ag	Cd	49	50	51	52	53	54
		In	Sn	Sb	Te	I	Xe
Au	80	81	82	83	84	85	86
		Tl	Pb	Bi	Po	At	Rn

⇒ AlN (6.28), AlP (2.45), AlAs (2.15), AlSb (1.63), GaN (3.44), GaP (2.27), GaAs (1.43), GaSb (0.70), InN (0.77), **InP (1.35)**, InAs (0.36), InSb (0.18)

⇒ **Tl** ← not used → **Bi**





1. General Properties of Semiconductors

1st Lecture

1.1. Qualitative Properties

Binary Compounds

Type	Elements	Bandgap (E_g) /eV
II-VI	ZnS	3.6
II-VI	ZnSe	2.7
II-VI	CdS	2.6
II-VI	CdSe	1.7
II-VI	CdTe	1.5

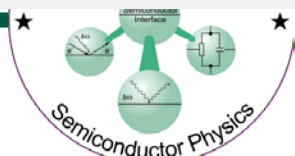


							0
							2
		IIIA	IVA	VA	VIA	VIIA	He
		5	6	7	8	9	10
		B	C	N	O	F	Ne
		13	14	15	16	17	18
		Al	Si	P	S	Cl	Ar
B	IB						
9	30	31	32	33	34	35	36
Cu	Zn	Ga	Ge	As	Se	Br	Kr
7	48	49	50	51	52	53	54
Ag	Cd	In	Sn	Sb	Te	I	Xe
9	80	81	82	83	84	85	86
Au	Hg	Tl	Pb	Bi	Po	At	Rn

⇒ ZnO (3.4), ZnS (3.68), ZnSe (2.7), ZnTe (2.26), CdS (2.48), CdSe (1.75), CdTe (1.43)

Mn → sometimes used

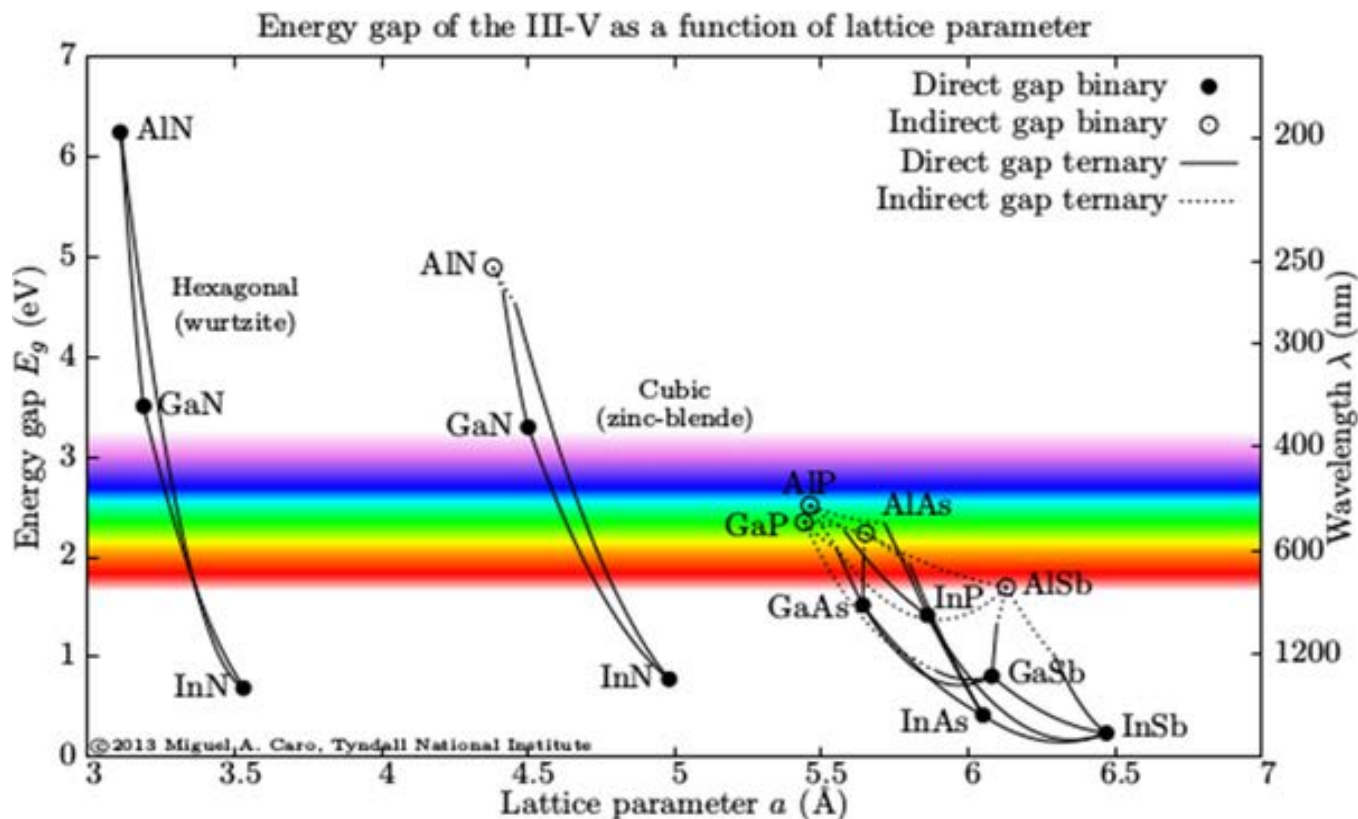
not used ← Po



Bandgap vs. Lattice constant

From binary to ternary compounds examples: AlGa₃N; AlGaAs; InGaAs

Semiconductor Master Graph



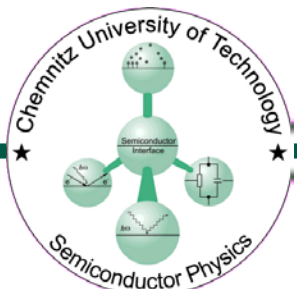
- ✓ Lines connecting two semiconductors indicate that some mixture of the two is possible, and how the lattice constant and the band gap will behave.
- ✓ The **GaAs - AsAl** case : the lattice constant does not change very much but the band gap changes from direct to indirect.
- ✓ The spectrum of light is schematically superimposed, to give some idea about the relation of the band gap energy to light color.

Oxides

- Most oxides are isolators;
- Current research in devolping semiconductor large band oxides for transparent electronics, e.g. ZnO, CuO, Cu₂O, Ga₂O₃.

Layered Semiconductors

- Binary compounds with layered crystal structures such as: MoS₂, MoSe₂, GaSe, etc;
- bonding within the layers is typically covalent and much stronger than the bonding between the layers;
- behavior of electrons in the layers is quasi-two-dimensional.



It looks like we have a great selection of semiconductors and their mixtures to choose from.

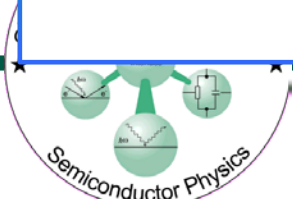
BUT

Choosing is one thing, making the semiconductor of your choice is something else.

This where semiconductor technology comes in.

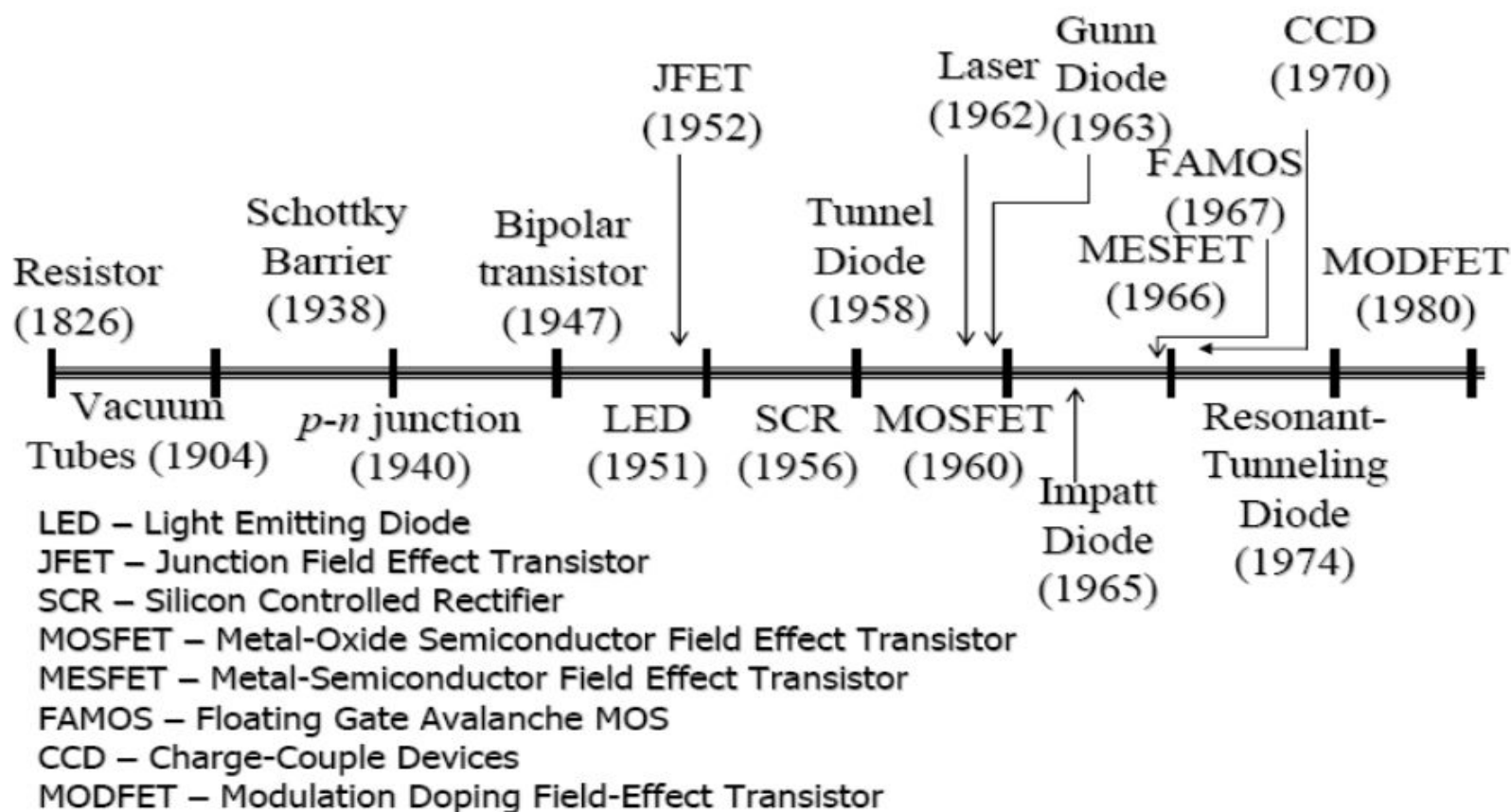
In reality, only a few of the many semiconductors shown in the Master Graph could be tamed to perform by now.

This is good news because it leaves something for us to do 😊 !



Applications as electronic components

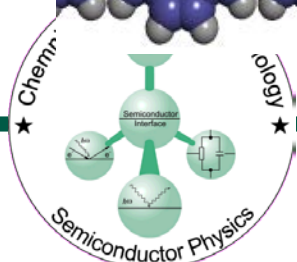
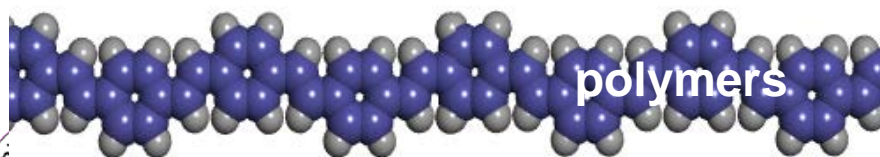
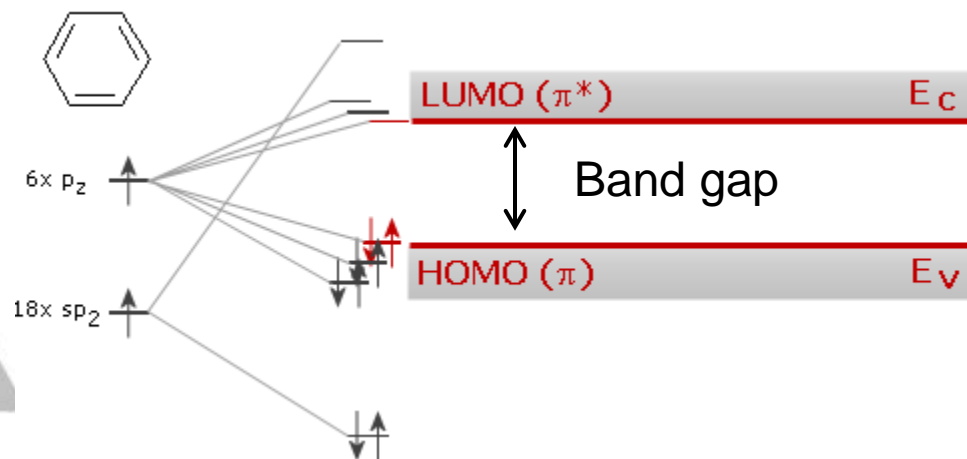
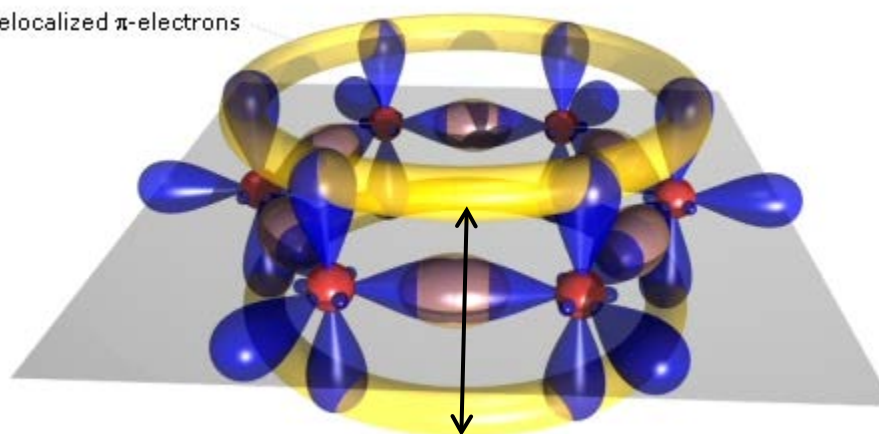
Semiconductor Materials



Organic Semiconductors

The **GAP** is between the highest occupied molecular orbital (**HOMO**) and the lowest unoccupied molecular orbital (**LUMO**).

delocalized π -electrons





OLEDs & OFETs

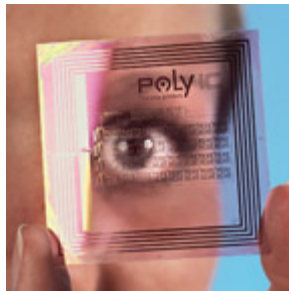
Displays

Lightning

RFID

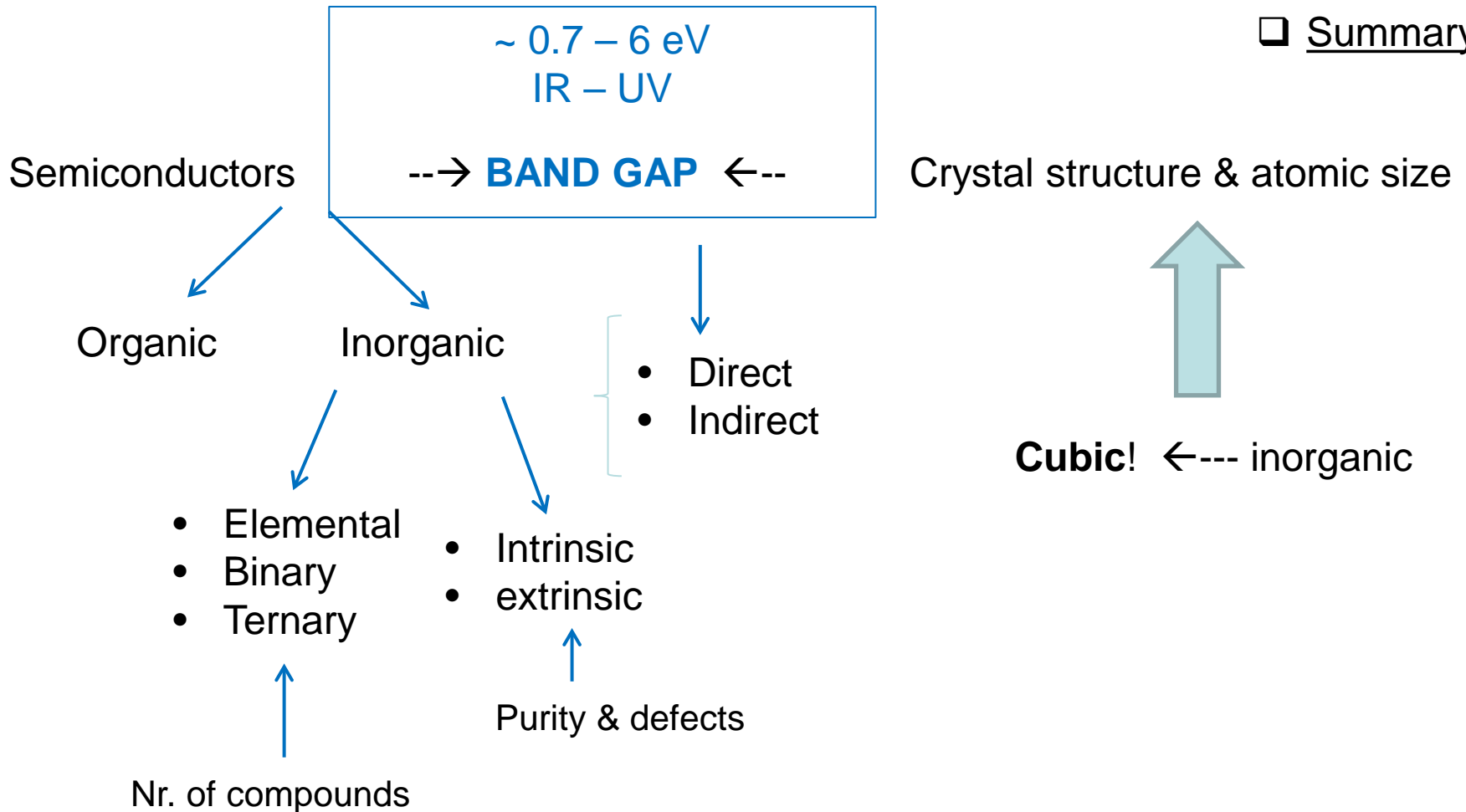
e-Paper

Organic Solar Cells



<http://www.slideworld.org/viewslides.aspx/Organic-Semiconductor-and-its-applications-ppt-2100090>

□ Summary



Covalent/ ionic bonding for binary and ternary compounds

Next lecture

CRYSTAL STRUCTURE