Physics of Materials

Dr. Thomas LaGrange

Masters Course PHYS-307

Fall 2025

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Course Organization

Lectures

- 12 Chapters, one chapter per week
- 13h15-15h on Friday
- The last lecture is on Dec. 13^{th}
- **No Lectures or exercises on Oct. 24^{th} – Autumn Break**

Exercises

- Not mandatory, but is recommended. Designed to reinforce lecture materials and their application
- 15h15-17h on Friday- no lecture; the last exercise session is on Dec. 20^{th}
- There will be **3** Electron Microscopy demonstrations/tours
(Today-September 12^{th}, October 17^{th} and November 21^{st})
- First part – review and questions on lectures and
- Second part –solutions of the previous week's exercises and questions on the current week's exercise

Moodle

- Schedule
- Course text and slides
- Additional reference materials for future studies and background information
- Exercises and solutions
- Group Communication- periodic emails and question forum

Course Exam Information and Format

- They will be individual Oral exams on an article chosen for your exam
- Oral exams are in-person in January, exact date TBA
- 30mins: 15-minute presentation and 15 minutes of questions on this article and other questions on the course.
- You can choose the articles, or I can suggest one for you.
- Articles must be submitted to me by Dec. 19th (last day of regular lectures for fall)
- The articles must be related to course content
- The presentation should focus on applying course theory to article data and interpretation, i.e., your slides should discuss the article's content in the context of the course materials.
- You can bring notes. The exam is an open book.
- My exam questions are still not hacked by ChatGPt

SCIENCE ADVANCES | RESEARCH ARTICLE

MATERIALS SCIENCE

Direct observation of individual dislocation interaction processes with grain boundaries

Shun Kondo,[1,2] Tasuku Mitsuma,[1] Naoya Shibata,[1,3] Yuichi Ikuhara[1,2,4,5]*

In deformation processes, the presence of grain boundaries has a crucial influence on dislocation behavior; these boundaries drastically change the mechanical properties of polycrystalline materials. It has been considered that grain boundaries act as effective barriers for dislocation glide, but the origin of this barrier-like behavior has been a matter of conjecture for many years. We directly observe how the motion of individual dislocations is impeded at well-defined high-angle and low-angle grain boundaries in $SrTiO_3$, via in situ nanoindentation experiments inside a transmission electron microscope. Our in situ observations show that both the high-angle and low-angle grain boundaries impede dislocation glide across them and that the impediment of dislocation glide does not simply originate from the geometric effects; it arises as a result of the local structural stabilization effects at grain boundary cores as well, especially for low-angle grain boundaries. The present findings indicate that simultaneous consideration of both the geometric effects and the stabilization effects is necessary to quantitatively understand the dislocation impediment processes at grain boundaries.

Historical Influence of Materials

Stone age - Prehistoric



Chalcolithic(copper) age (>4000 BC)

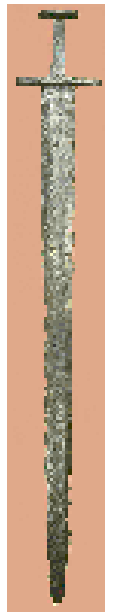



Bronze (copper+12%tin) age (~3000 BC)



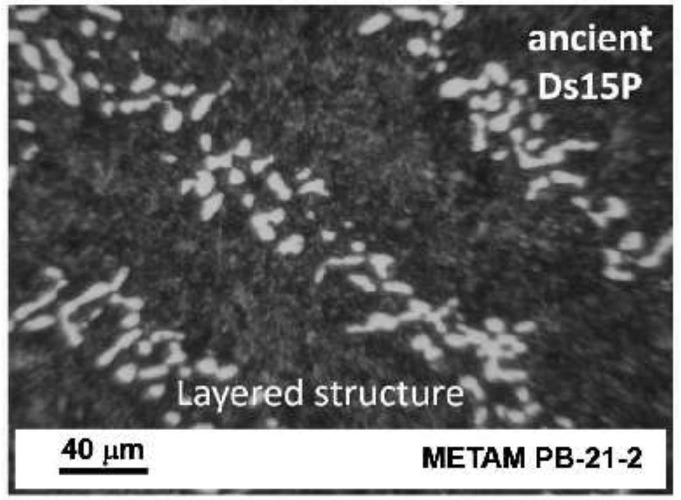

First alloy used

Iron age (2000 BC-1600s)

Revolutionized Warfare and farming

Weaponry and Warfare



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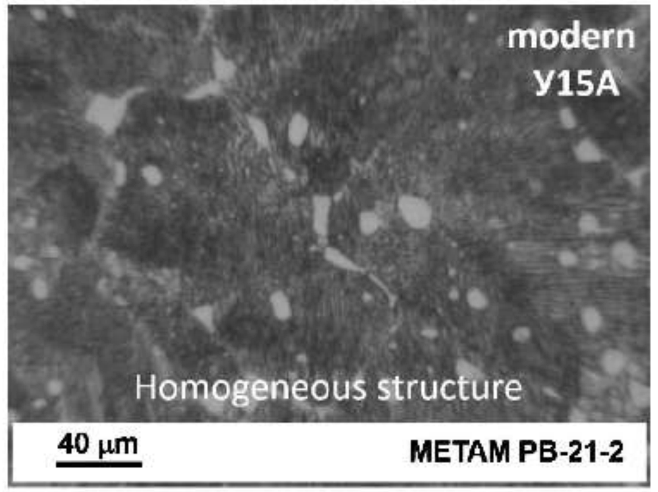

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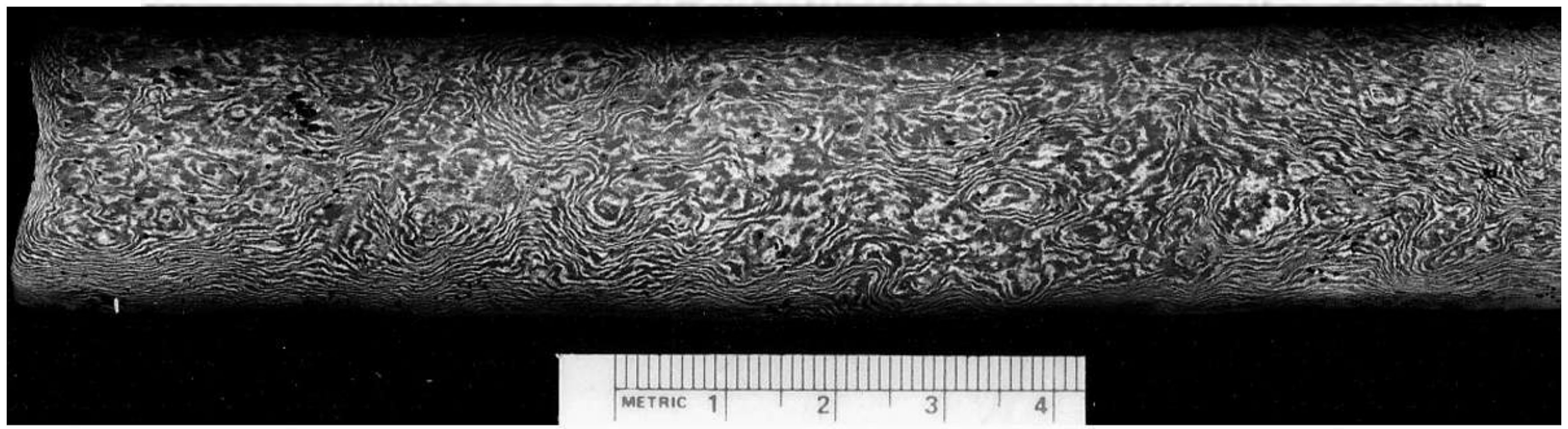

The Figiel blade purchased in Rajasthan India.

Writings found in Asia Minor said that to temper **Damascus** sword, the blade must be heated until it glows "like the sun rising in the desert. " It then should be cooled to the color of royal purple and plunged "into the body of a muscular **slave**" so that his strength would be transferred to the sword

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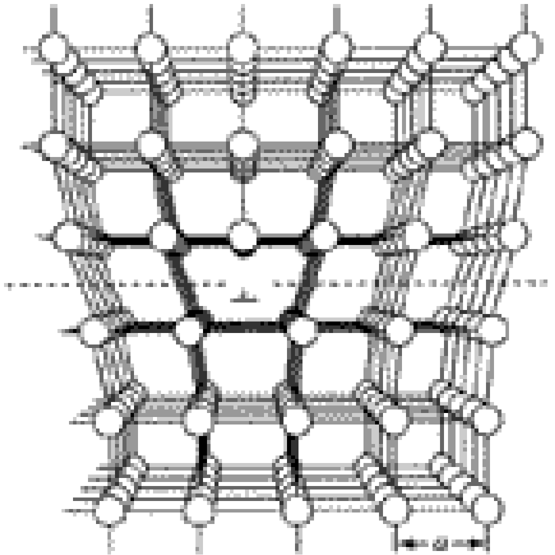
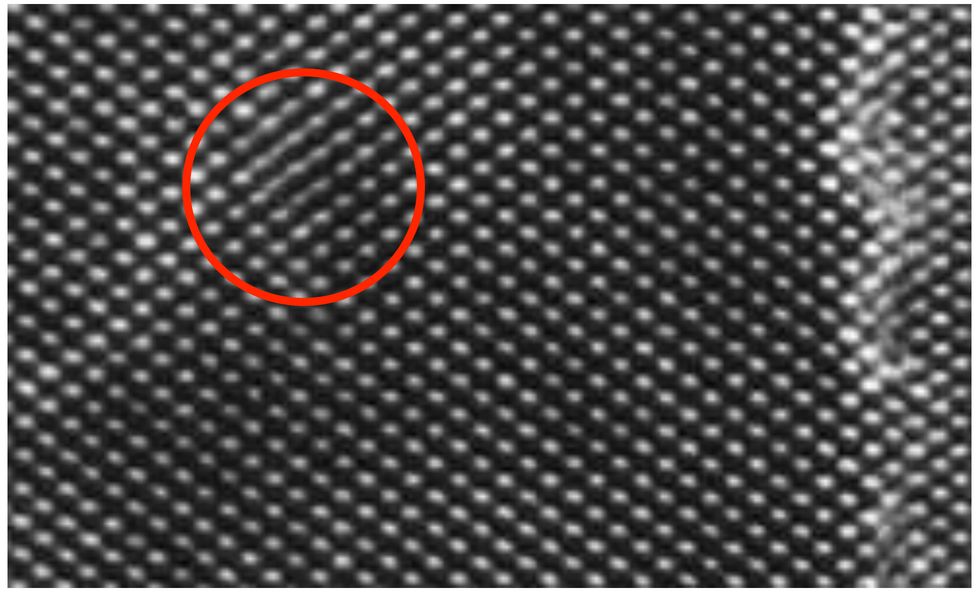
Metals and 20th-century science

dislocations



1934 Taylor, Polanyi, Orowan

1956, JP Hirsch



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Turn of the Century: Era of Internet and dot.com

COMMENTARY

The science of dirt

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e-mail: rwc12@cam.ac.uk

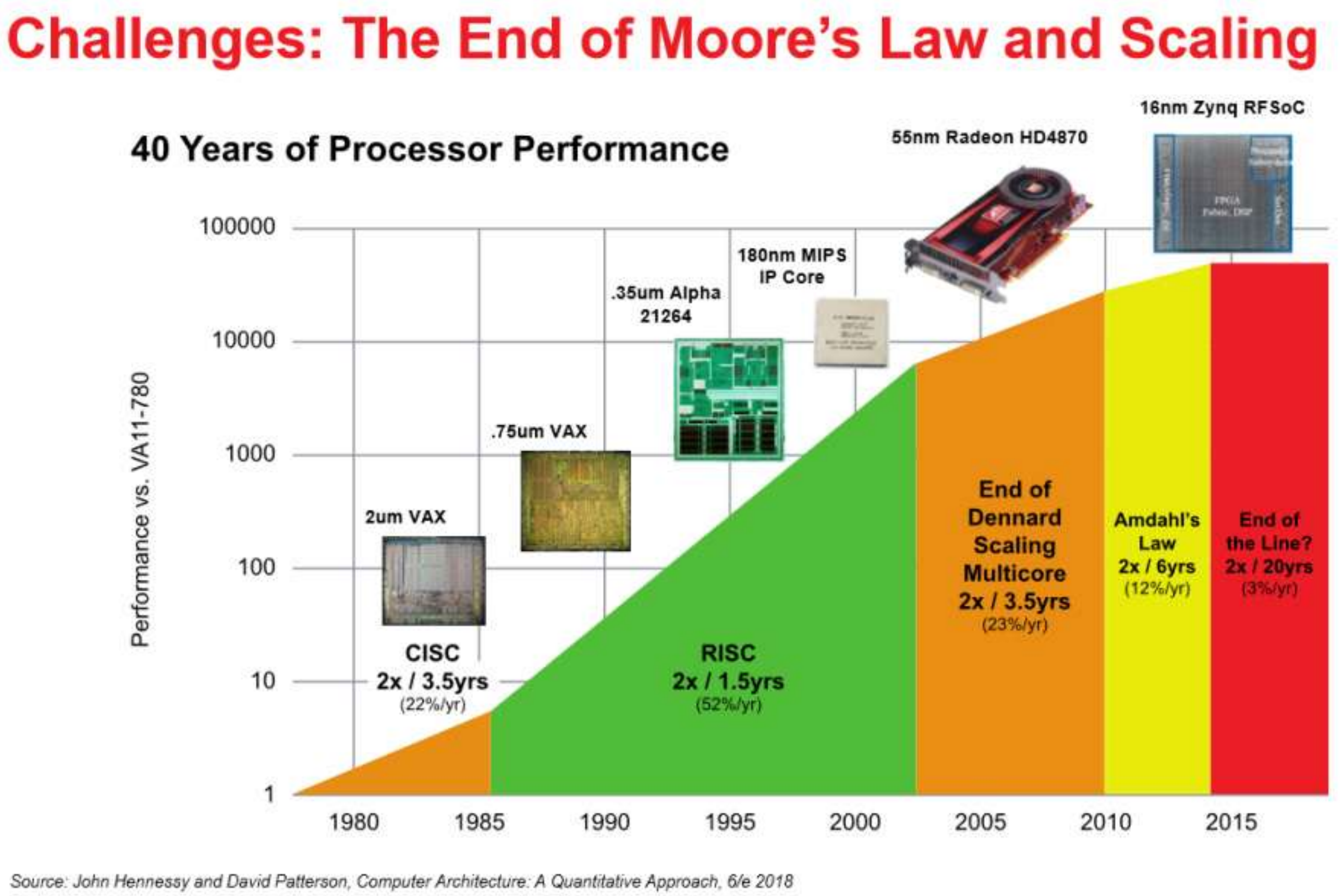
Economics is often called the dismal science, but to many outsiders materials research is still the dirty science. Robert Cahn explains why materials scientists should be proud of their history.

Tracing the roots of materials science is, much as for any other discipline, an undertaking fraught with pitfalls. Those who research the origins of scientific disciplines are inclined to search for the 'founders' of those disciplines, Newton as the father of physics say, or Lavoisier as the father of chemistry. Despite this tendency, in reality all disciplines have multiple founders; it is just a question of which aspects of a discipline are judged to be the most central. The historian of 'materials science' need only look back to the late 1950s, when the term first entered into common usage, to encounter Morris Fine of Northwestern University, Chicago, who fought successfully to introduce the concept into the university teaching there in 1958.

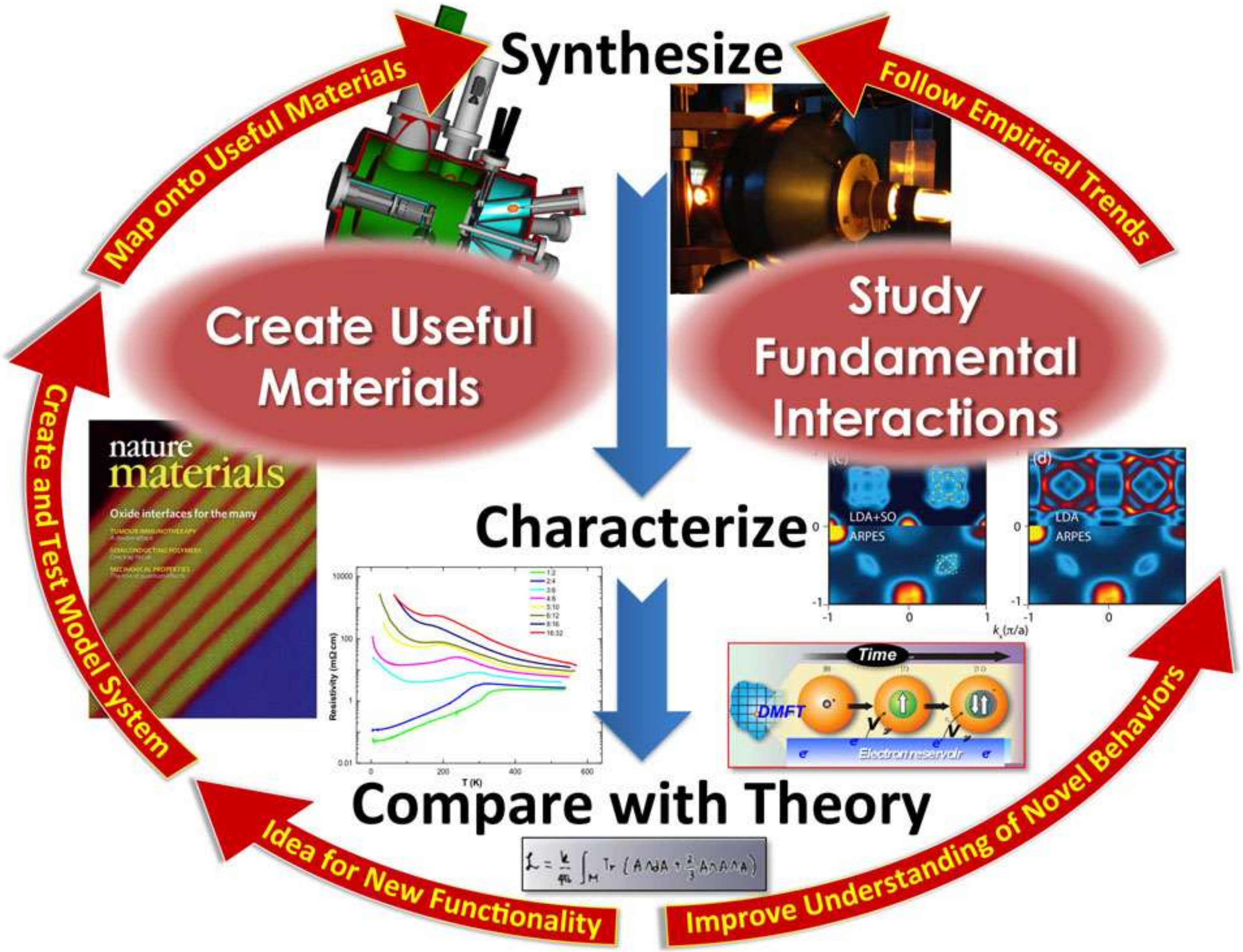
In US industry, at about the same time, a hyperactive research manager for General Electric Corporate Research Center in New York State — Herbert Hollomon — organized a brilliantly successful research group based on the broad concept of materials science. In 1958, Hollomon wrote: "Out of metallurgy, by physics, comes materials science." He was not alone. William Baker of Bell Laboratories in Murray Hill, New Jersey, another early protagonist of materials science, had learnt a valuable lesson from the development of the transistor at the institute a decade earlier — without the close collaboration of physicists,

Nature Materials(2002)

Silicon age



Materials by Design



Theoretical correlations between defects (Dislocations) and mechanical behavior

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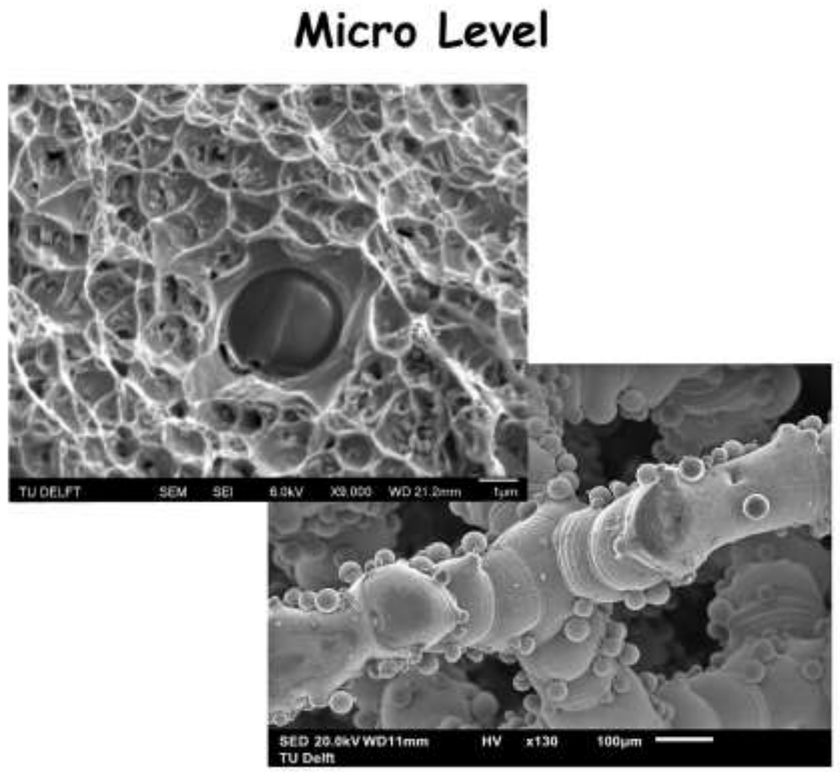
Additive Manufacturing (3-D printing)



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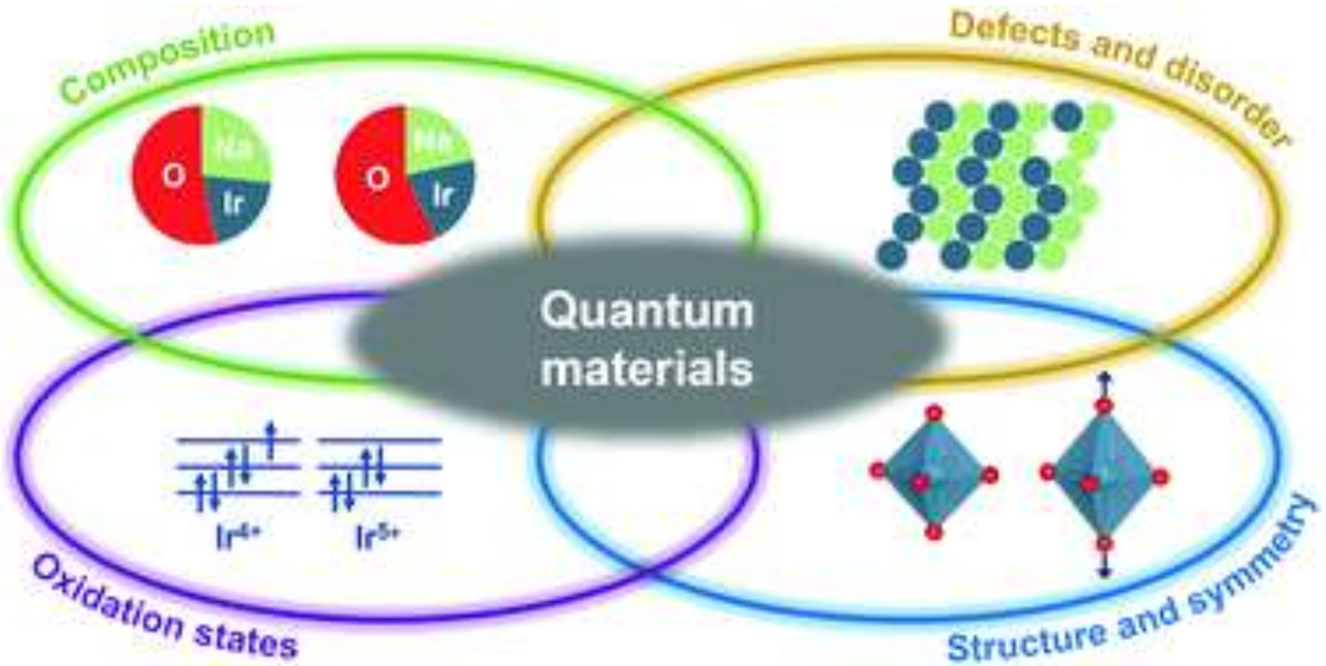
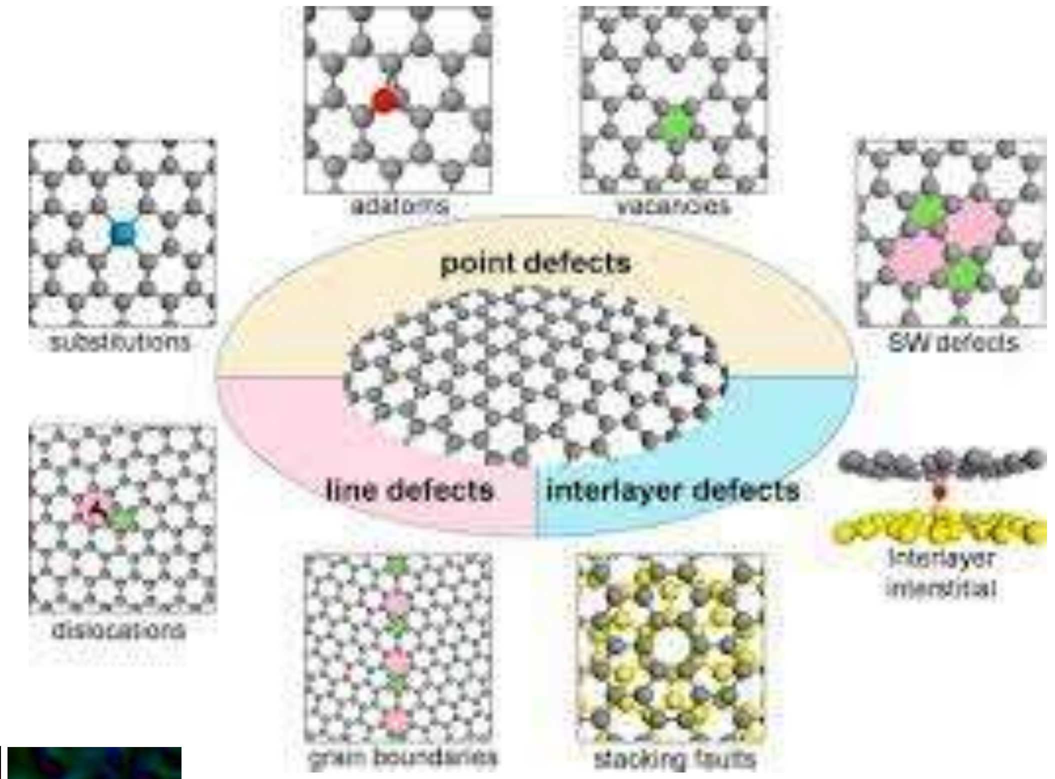
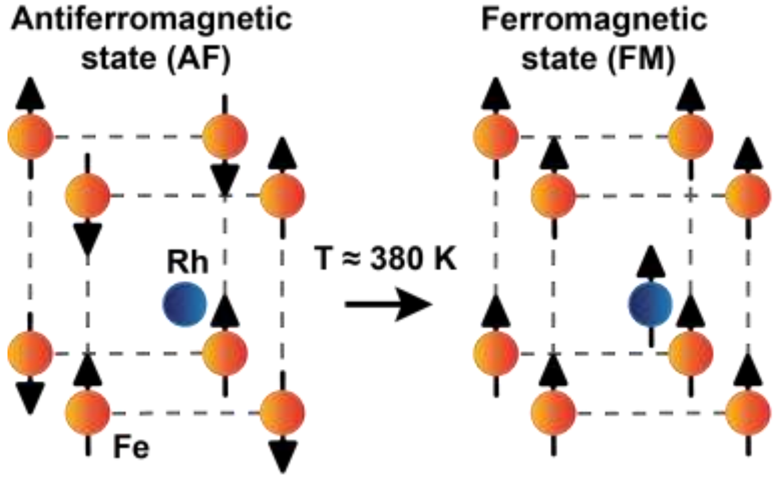
Quantum materials



Defects in 2-D materials

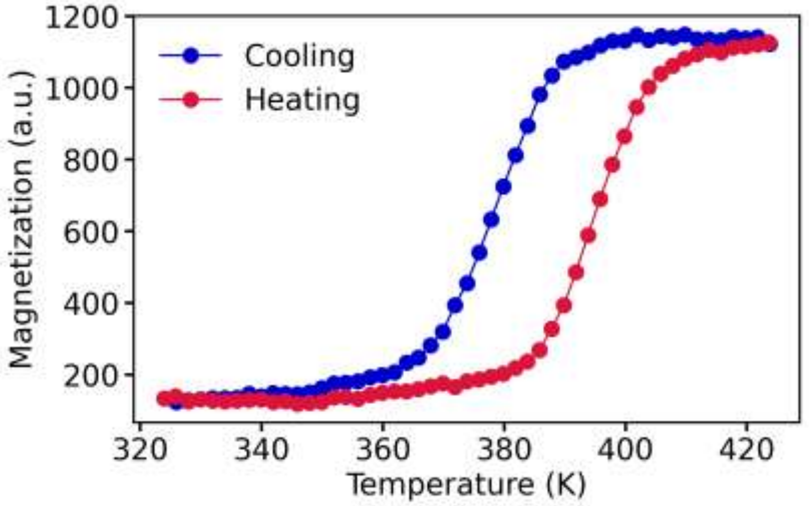


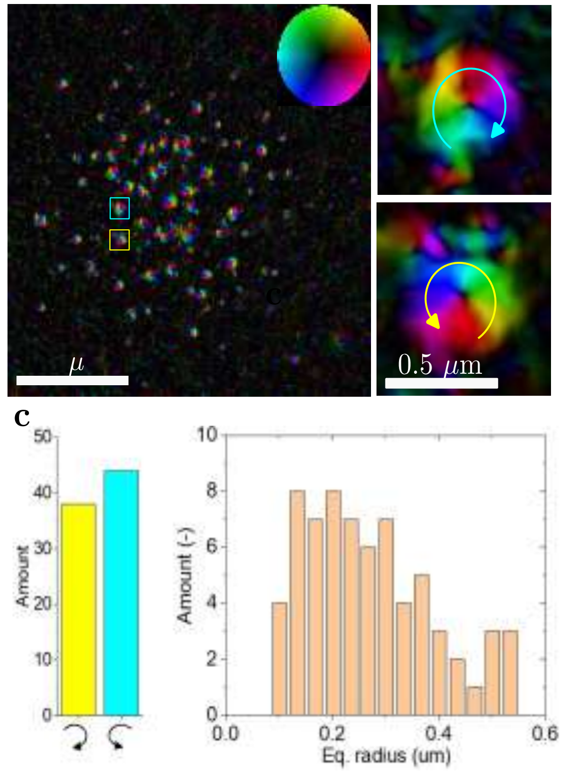


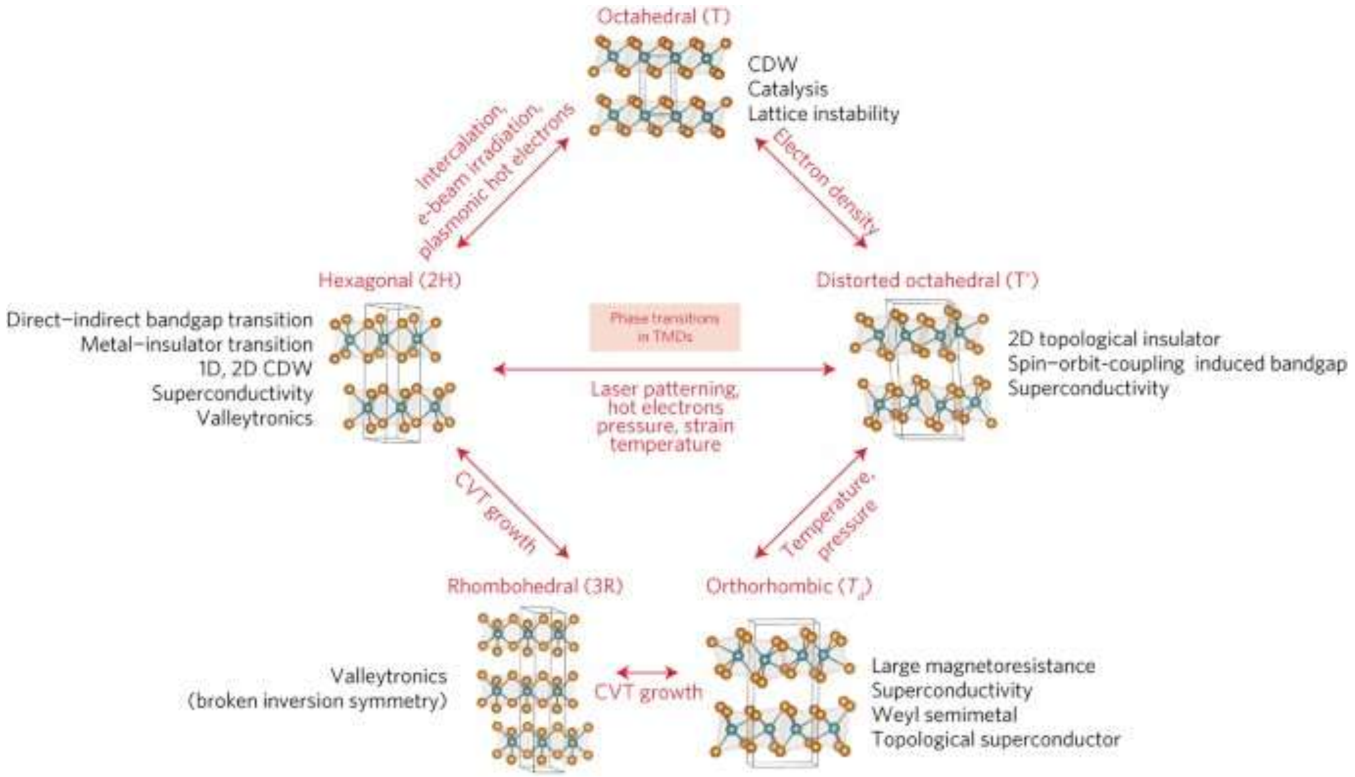
Fe_xRh_{1-x}; x ∈ (0.48; 0.52)

Phase transitions

Coexistence of AF-FM phases







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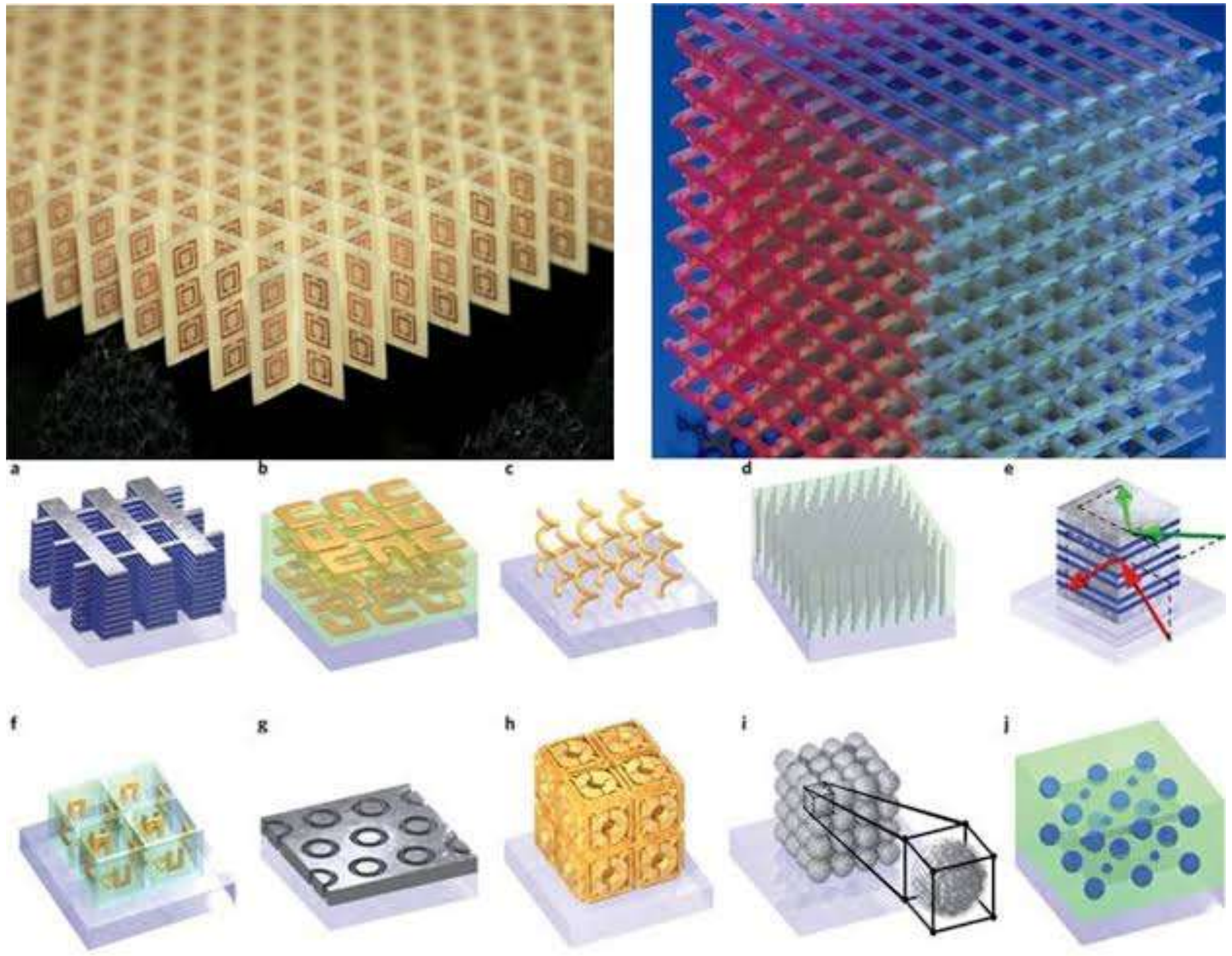
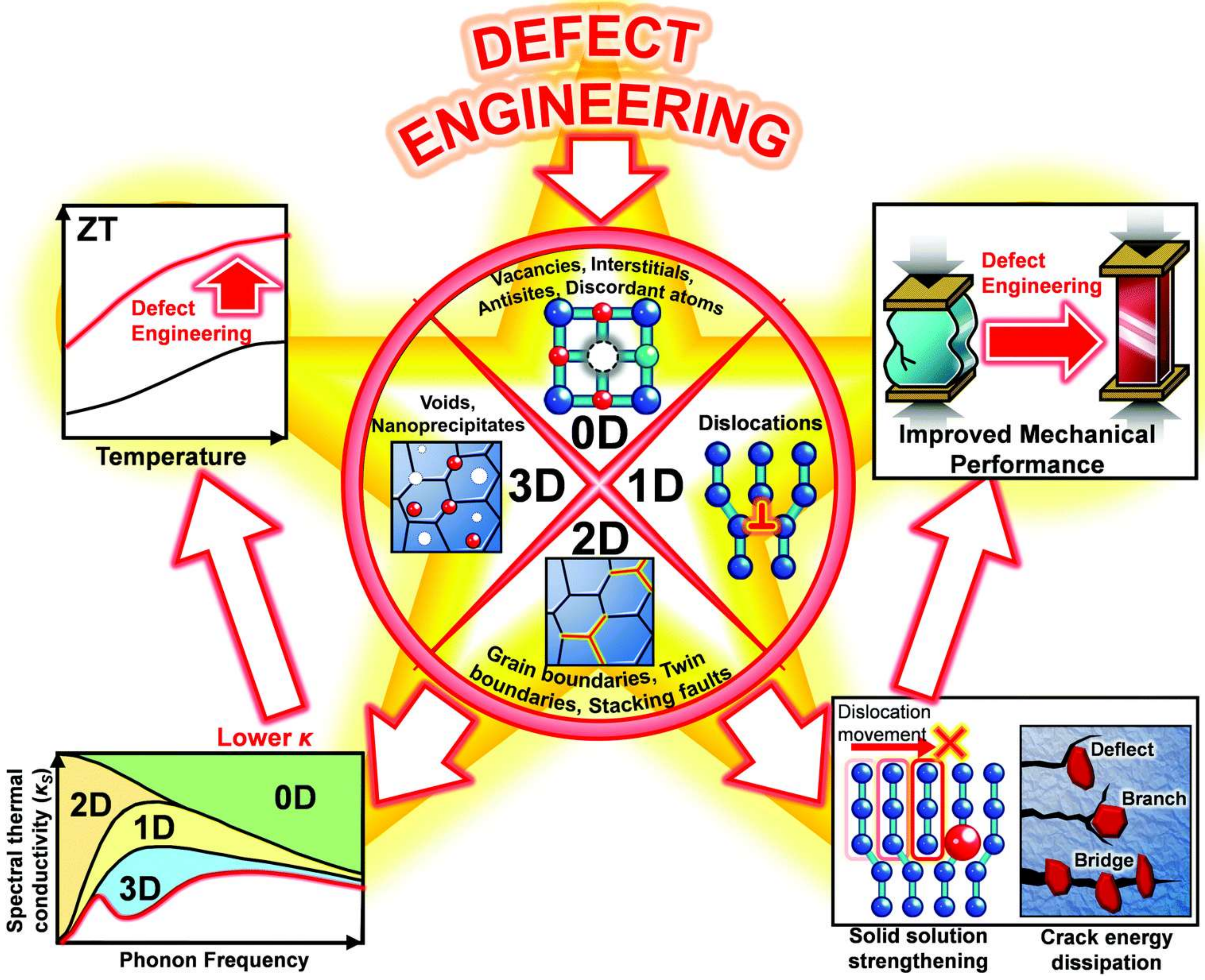
Metamaterials and defect engineering



Materials designed for light manipulation of their mechanical, electronic, or magnetic properties



Course Outline

This course builds a bridge from atomic-scale structure to macroscopic properties:

- **Chapters I–II**: Foundations — atomic bonds and crystal structures.
- **Chapter III**: Theory of elasticity, linking atomic interactions to macroscopic deformation.
- **Chapters IV–X**: Defects in crystals, defect diffusion kinetics, dislocation theory, and experimental characterization, explaining how imperfections govern plasticity, strength, and toughness.
- **Chapters XI–XII**: Phase transformations — solidification, martensite, and recrystallization — showing how processing controls microstructure and performance.

Core Learning Goals:

- Interpret the **mechanical behavior of solids** from their **atomic structure**,
- Understand the role of **defects and microstructure**
- Theoretical understanding of **phase transformations**
- Appreciate the central role of materials in technology and innovation.

EPFL

Dr. Thomas LaGrange

Chapter 1: Atomic bonding

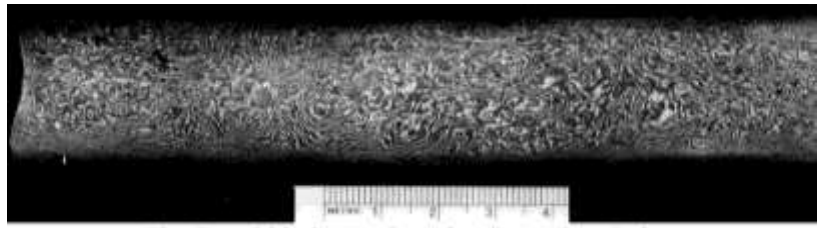
LUMES

Masters Course PHYS-307

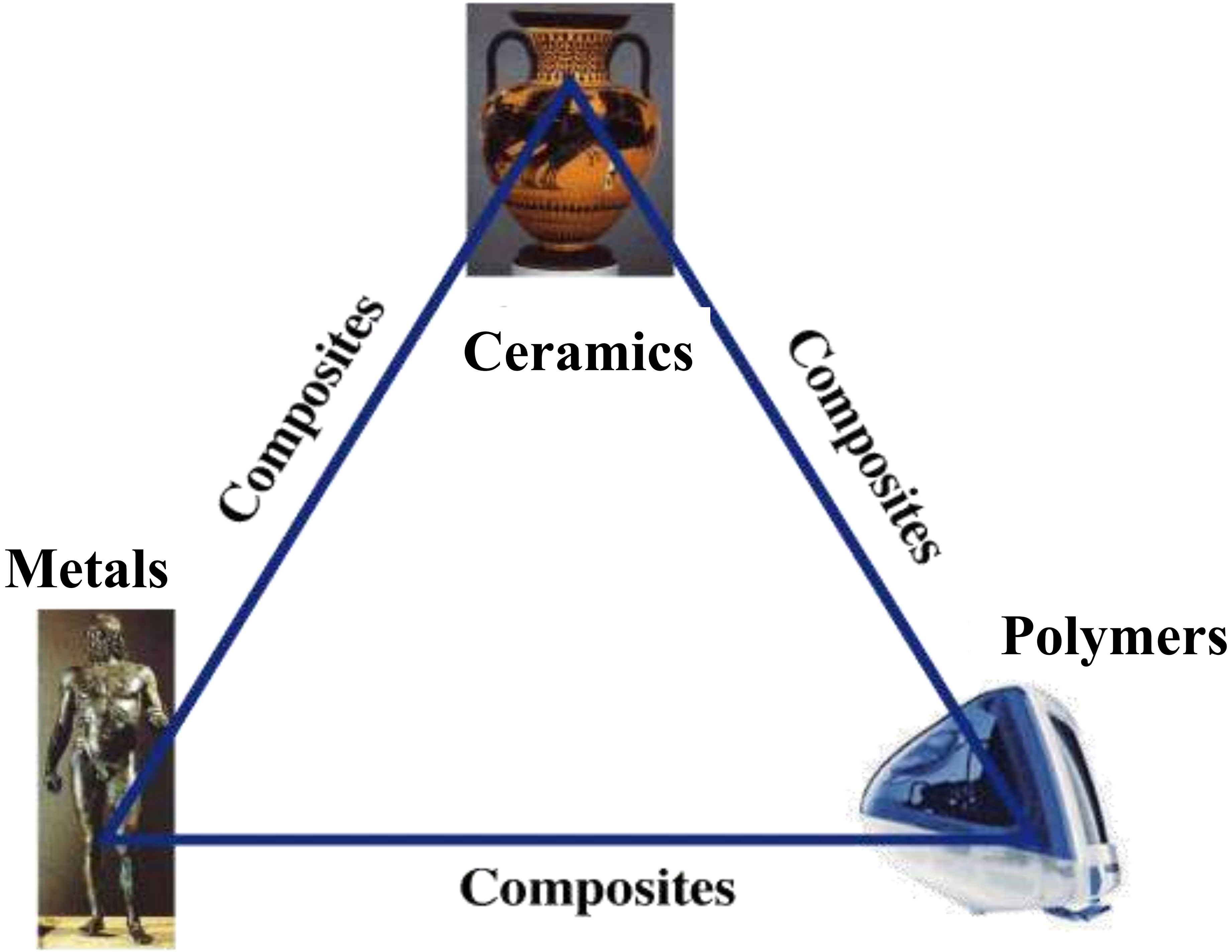
Fall 2024

Families of materials

Glasses



The Figiel blade purchased in Rajasthan India.



Diamond

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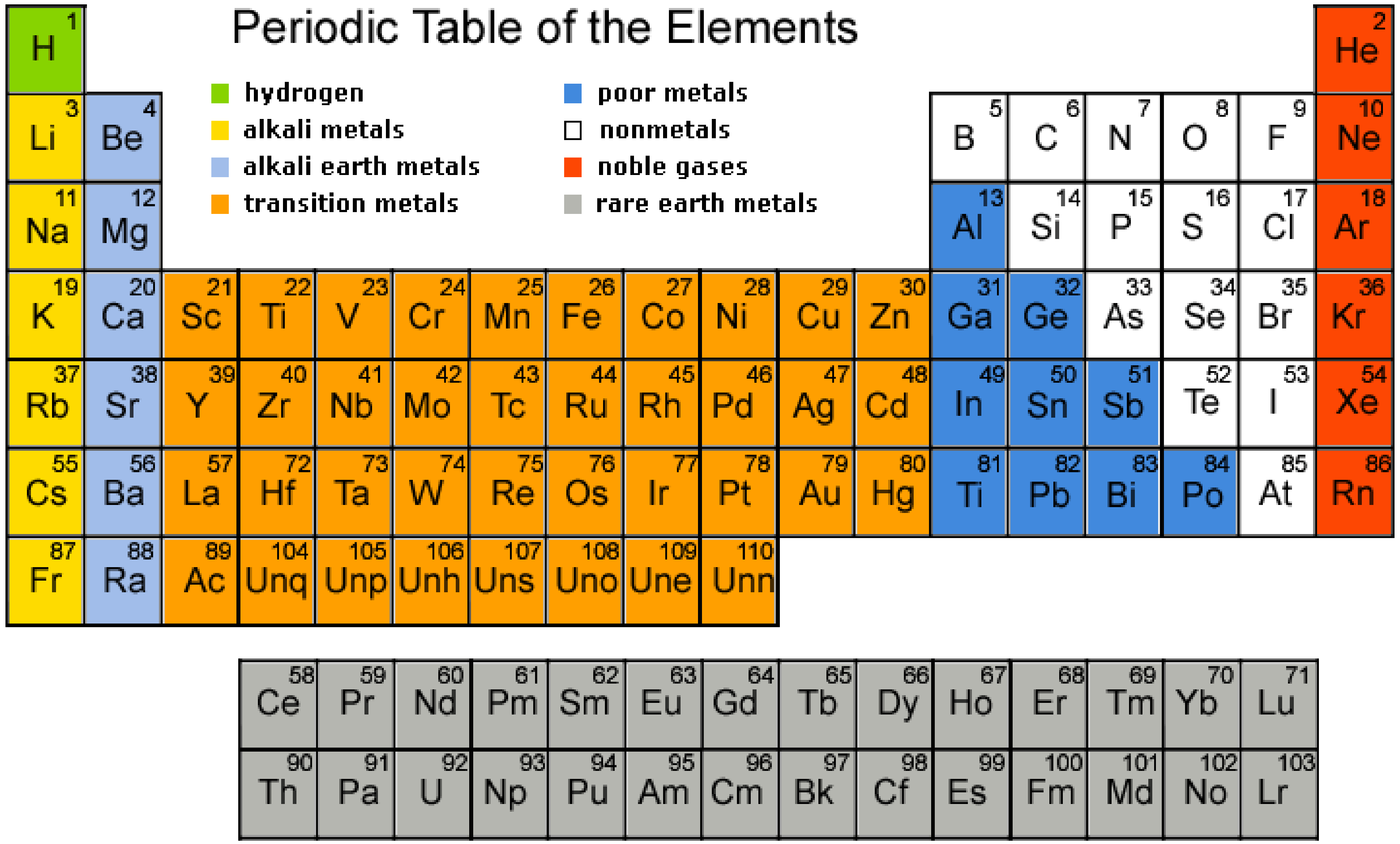
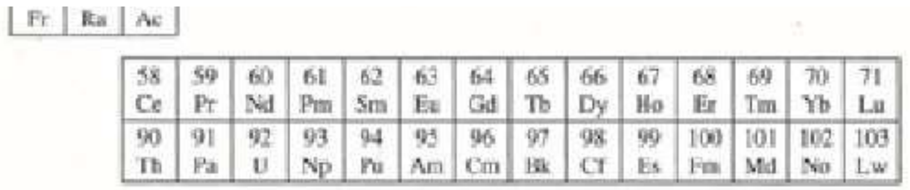
Metals





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Atomic bond

$$E_C = (E_{at.free} - E_{at.bonded})$$

$$(H_0 + H_1) \cdot \psi = (E_0 + \Delta E) \cdot \psi$$

Perturbation

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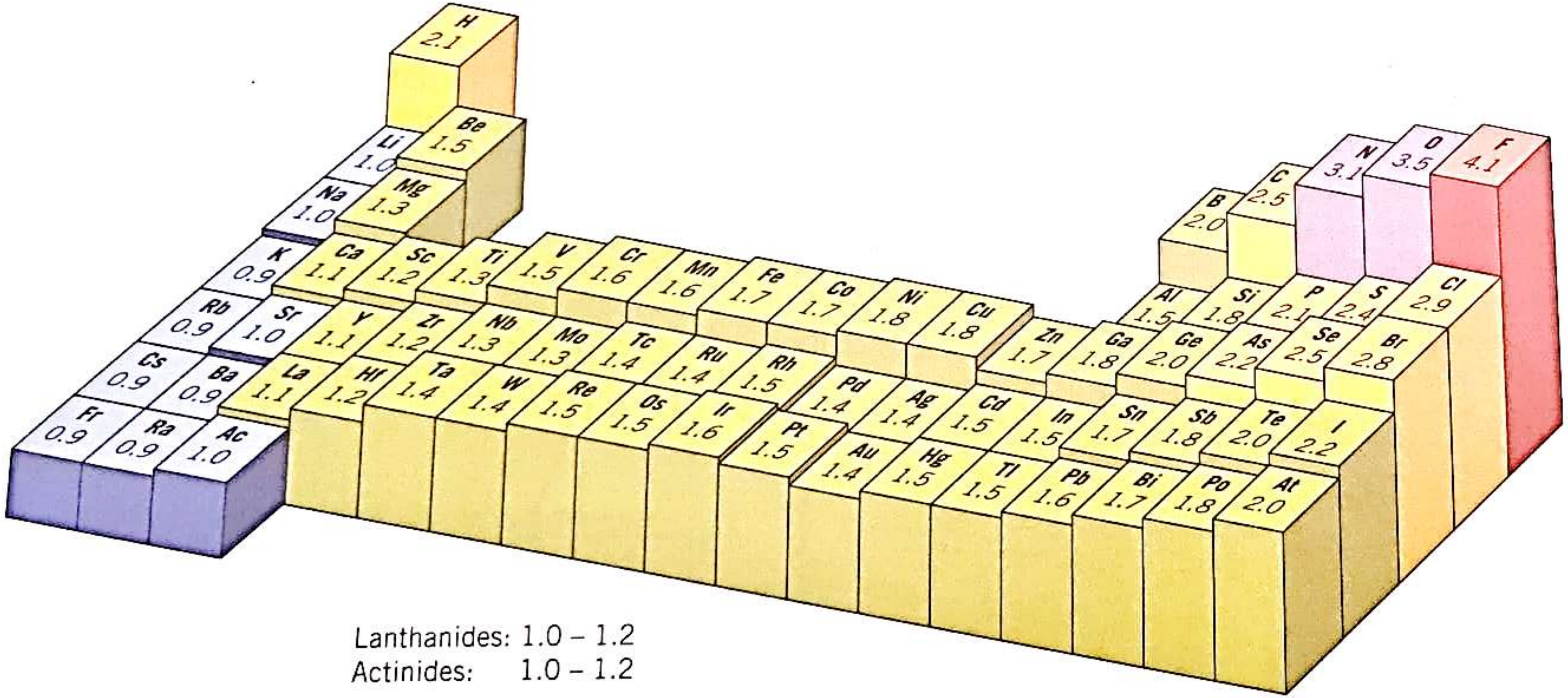
Ionic bond



Electronegativity

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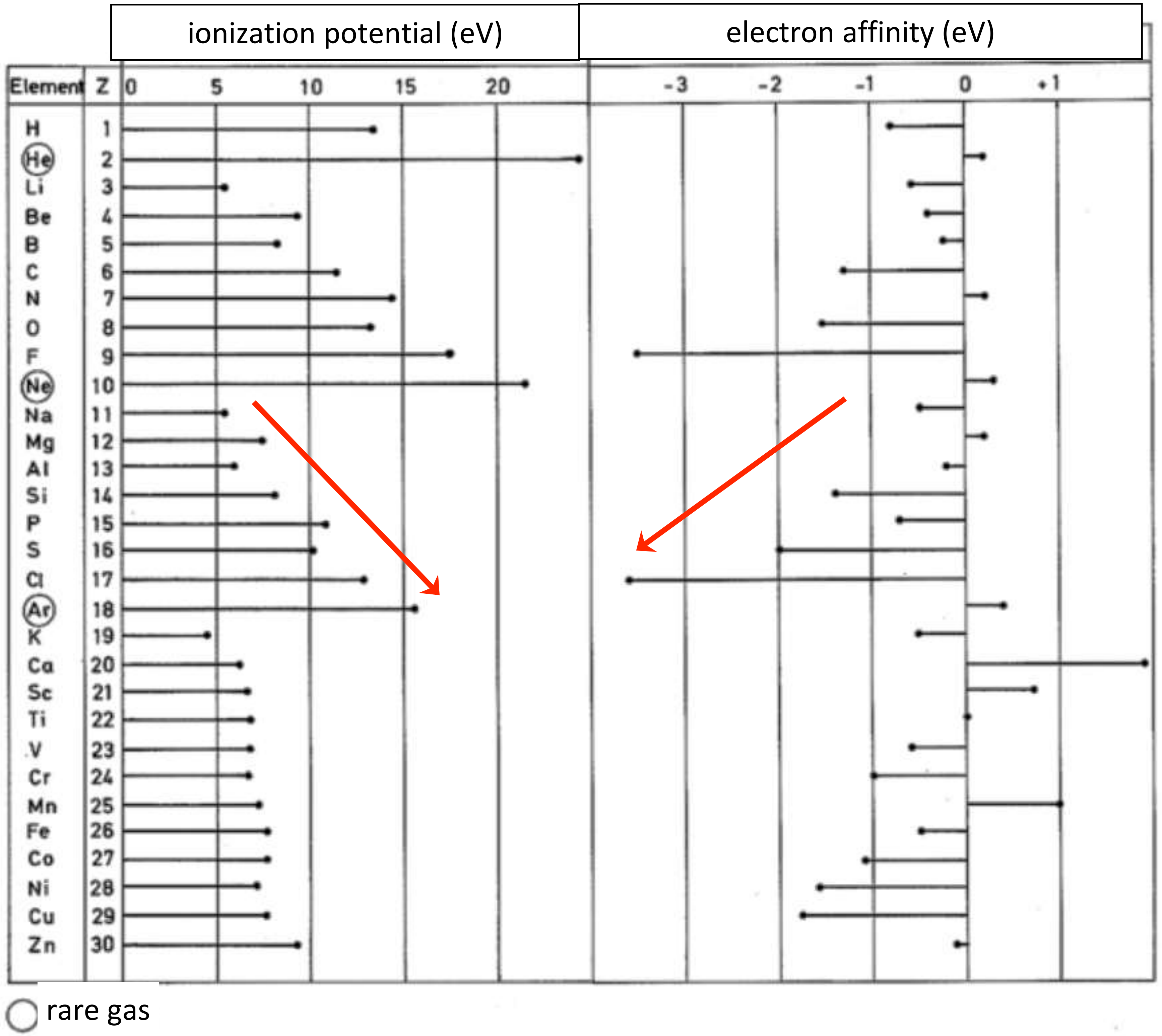
Ionic bond



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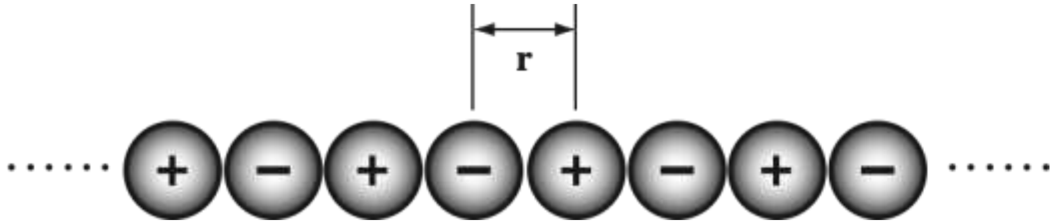
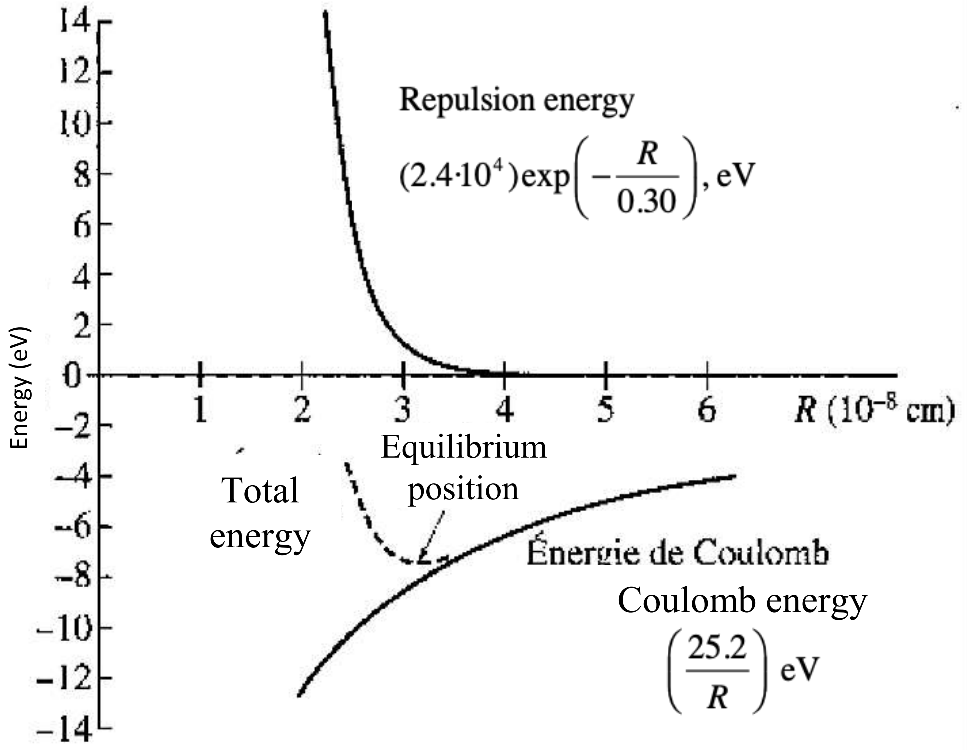
Ionic bond



$$U_i = \sum_j U_{ij}$$

$$U_{ij} = \lambda \exp((-r_{ij})/\rho) \pm \frac{q^2}{4\pi\varepsilon_0 r_{ij}}$$



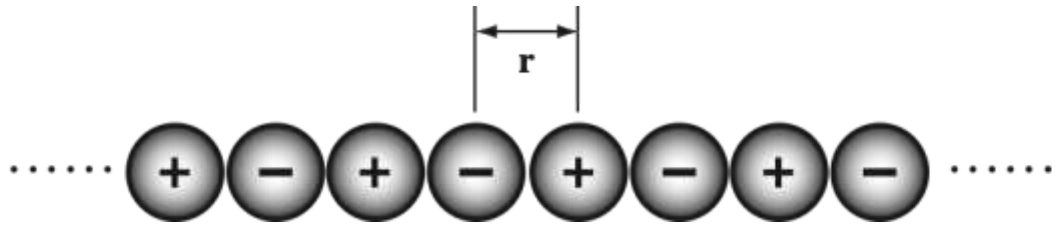
Energy (per molecule) of the KCl crystal, showing the Madelung and repulsion contributions

ρ compressibility constant
q electron charge
ϵ_o permittivity
r_{ij} distance between ions i - j
z atomic number
R average radial spacing of ions
λ is constant

$$\sum_j \lambda \exp((-r_{ij})/\rho) = \lambda z \exp(-R/\rho)$$ Repulsion term

Coulombic term $$\sum_j \pm \frac{1}{r_{ij}} = \frac{\alpha}{R}$$ α is the Madelung constant

Ionic bond



$$U_i = \left(z\lambda e^{-R/\rho} - \frac{\alpha q^2}{4\pi\varepsilon_0 R} \right)$$ N bonds

$$\frac{dU_i}{dR} = 0 \longrightarrow R_0$$ Equilibrium ion spacing

$$E_c = U_{tot} = -\frac{N\alpha q^2}{4\pi\varepsilon_0 R_0}\left(1 - \frac{\rho}{R_0}\right) \qquad \frac{\rho}{R_0} \approx 0.1$$ For solids

$$E_B = E_c + E_I + E_A$$

E_c=coulombic energy
E_I= ionization energy
E_A= electron affinity

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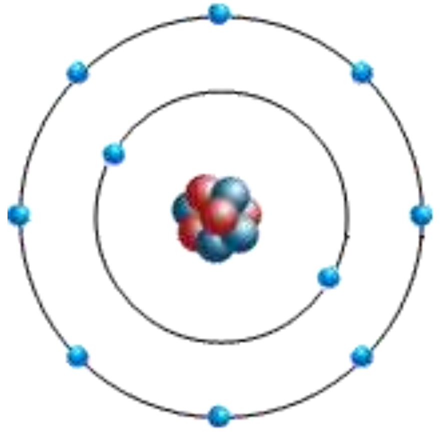
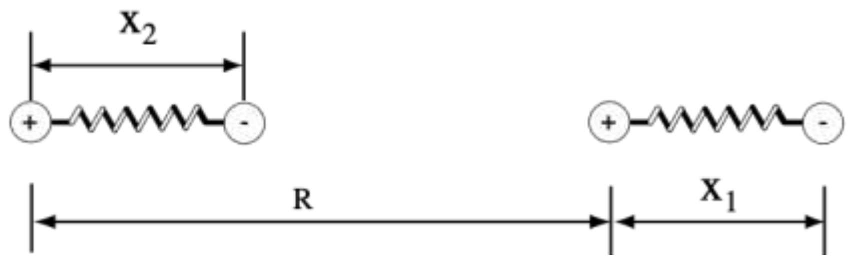
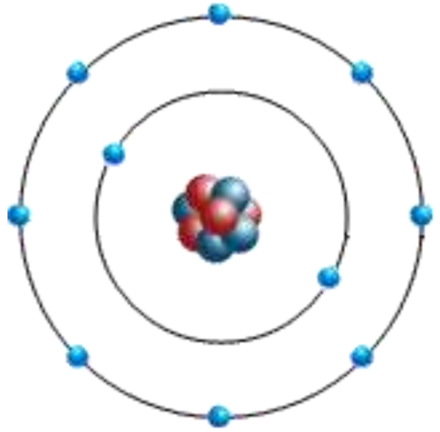
Van der Waals interaction



Electron dipole interactions





$$H_0 = \frac{1}{2m} p_1^2 + \frac{1}{2} k x_1^2 + \frac{1}{2m} p_2^2 + \frac{1}{2} k x_2^2$$

$$(H_0 + H_1)\cdot\psi = (E_0 + \Delta E)\cdot\psi \qquad h\omega_0 \qquad \omega_0 = \sqrt{k/m}$$

Solve for eigenvalues

$$\Delta E = -h\omega_0 \frac{1}{32\pi^2\varepsilon_0^2}\left(\frac{e^2}{kR^3}\right)^2$$

R/σ is a constant at equilibrium, i.e., $\frac{dU}{dR} = 0$

	Ne	Ar	Kr	Xe
R/σ	1.14	1.11	1.1	1.09

Lennard-Jones

$$U = \left(\frac{A}{R^{12}} - \frac{B}{R^6}\right) = 4\varepsilon\left[\left(\frac{\sigma}{R}\right)^{12} - \left(\frac{\sigma}{R}\right)^{6}\right]$$

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

F.C.C. structure

$$\sum_{ij}\left(\frac{1}{p_{ij}}\right)^{12} = 12.13188$$

$$\sum_{ij}\left(\frac{1}{p_{ij}}\right)^{6} = 14.45392$$

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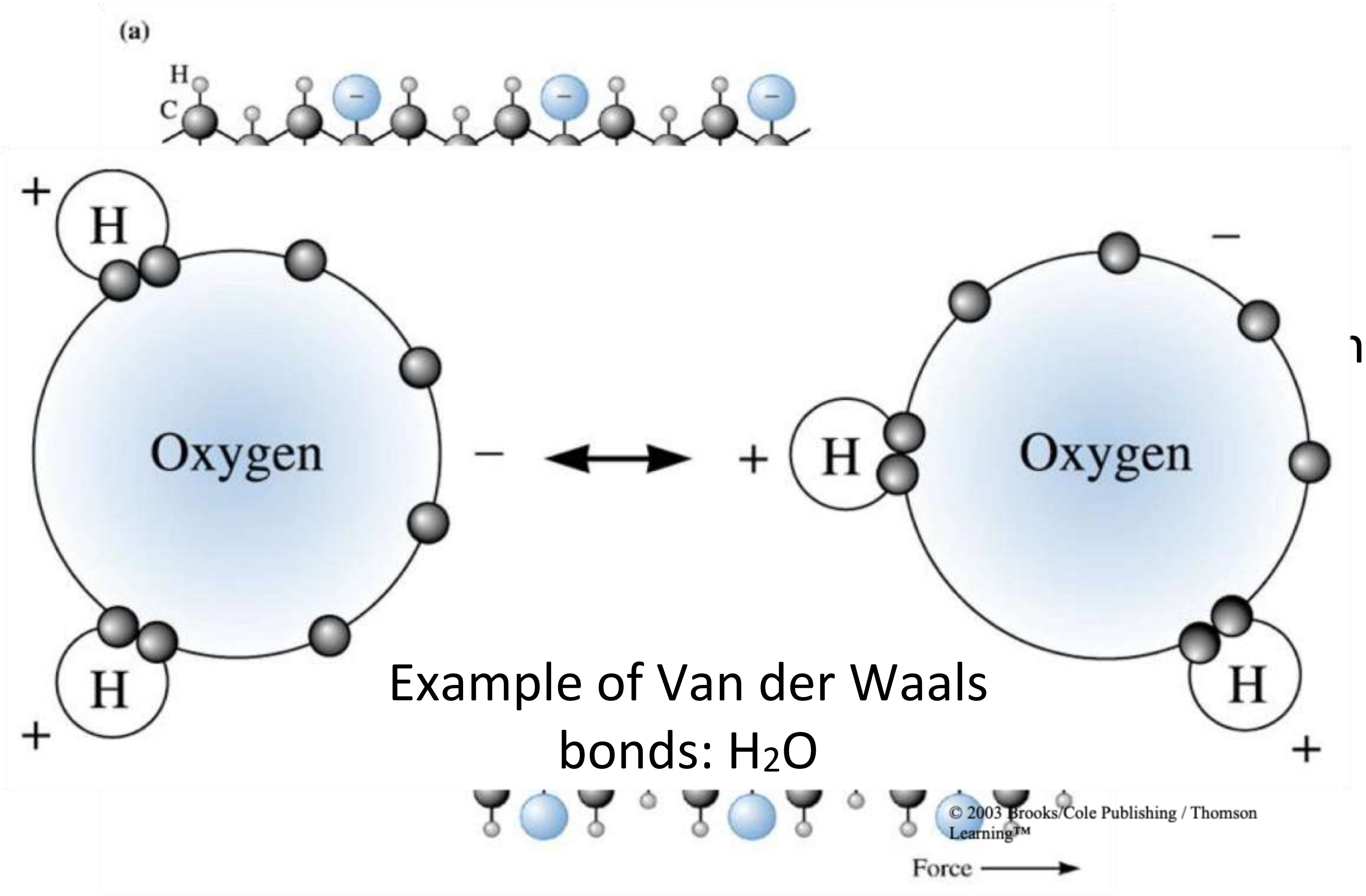
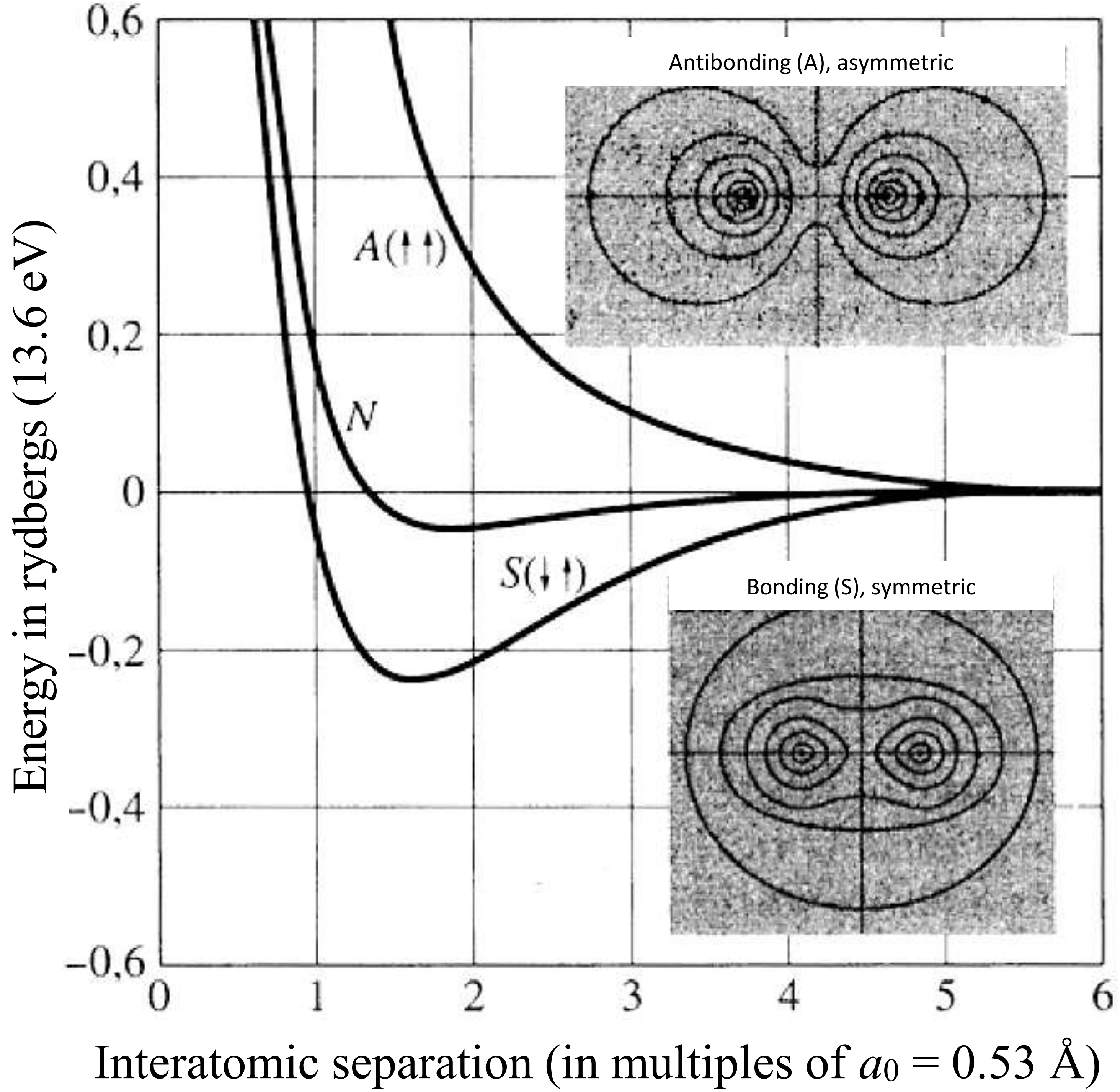
Van der Waals interaction

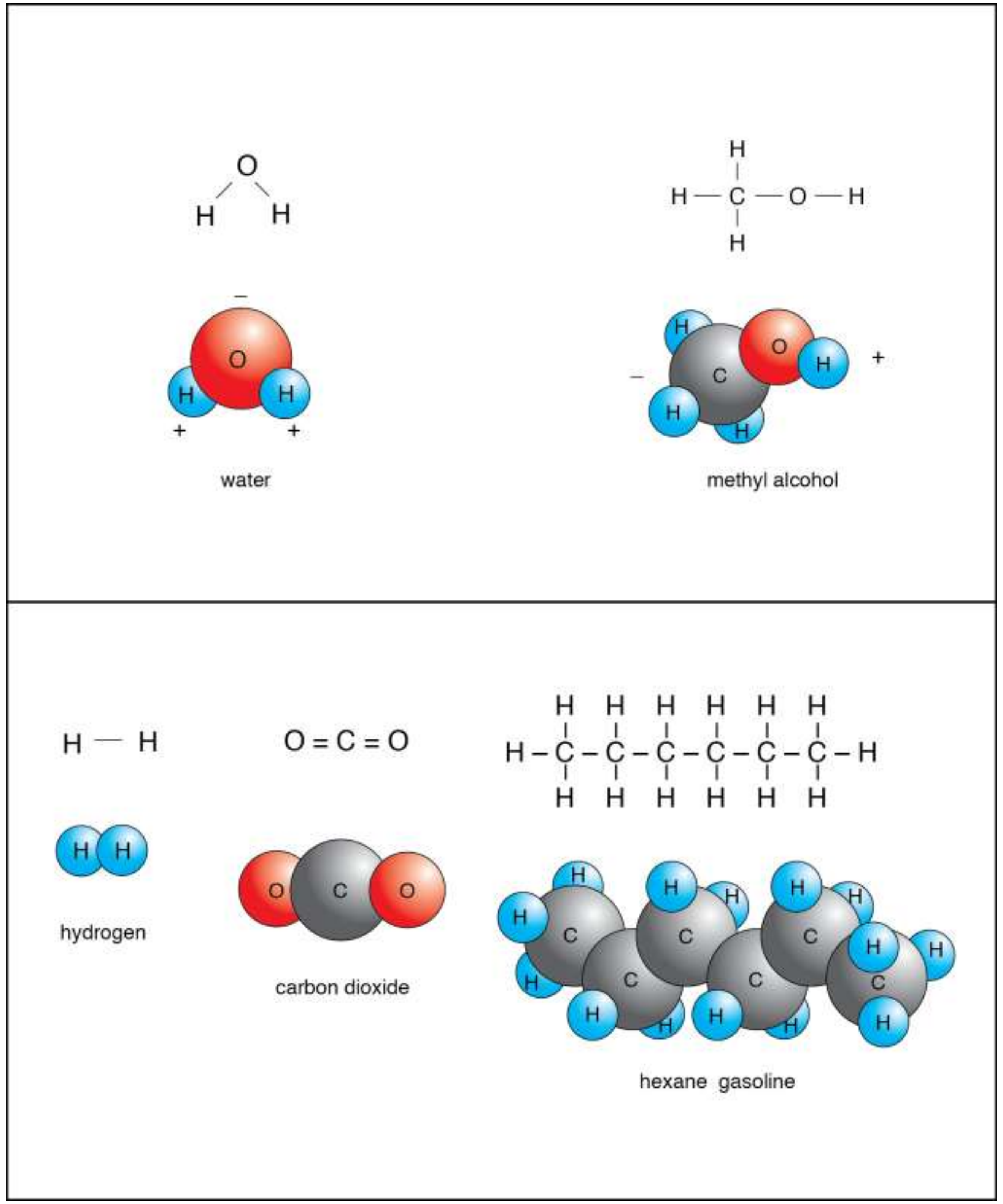


Example of Van der Waals bonds: H_2O

Covalent bond



Why do covalently bonded compounds tend to have low densities?

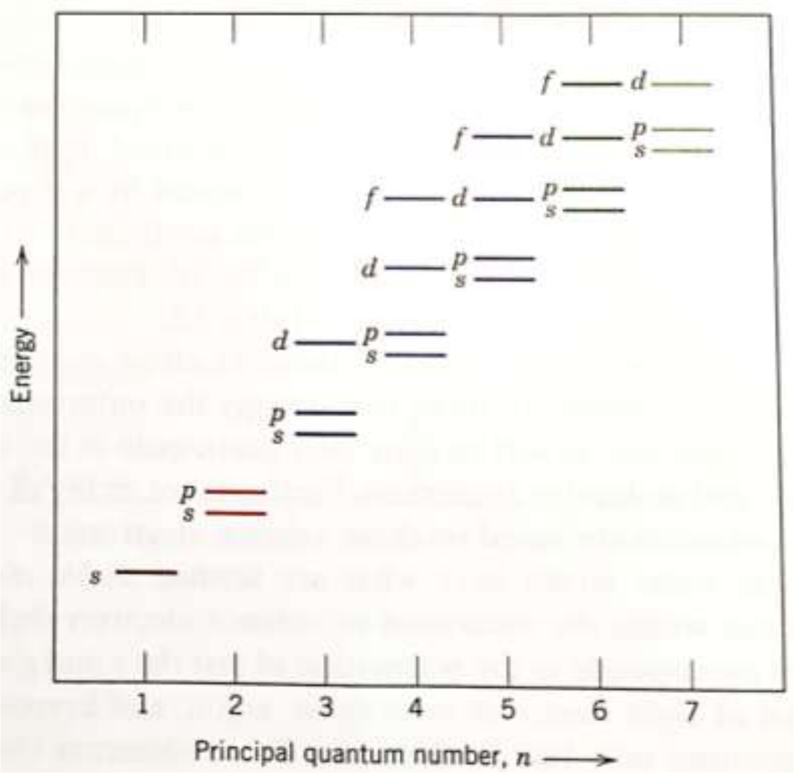


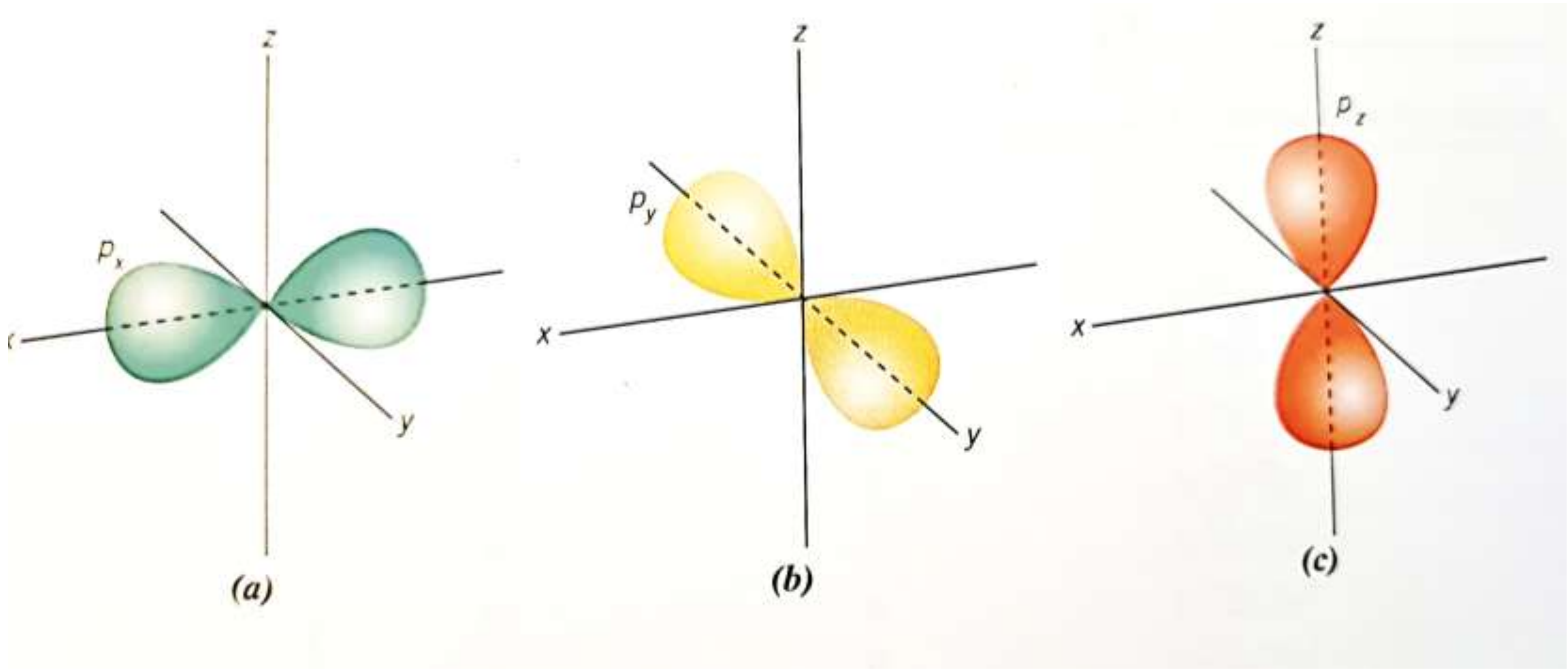
- Atomic packing is low due to directional bonding
- Unit cell dimensions are larger
- Thus, densities tend to be lower

Molecule	Bond Type	Molecular Shape	Molecular Type
Water	δ- O–H δ+ Polar Covalent	δ+ H, δ+ H, O δ- Bent	Polar
Methane	C–H Non-Polar Covalent	Tetrahedral	Non-Polar
Carbon Dioxide	δ- O=C δ+ Polar Covalent	O=C=O Linear	Non-Polar

Covalent bond

Value of n	Value of l	Values of m_l	Subshell	Number of Orbitals	Number of Electrons
1	0	0	1s	1	2
2	0 1	0 -1,0,+1	2s 2p	1 3	2 6
3	0 1 2	0 -1,0,+1 -2,-1,0,+1,+2	3s 3p 3d	1 3 5	2 6 10
4	0 1 2 3	0 -1,0,+1 -2,-1,0,+1,+2 -3,-2,-1,0,+1,+2,+3	4s 4p 4d 4f	1 3 5 7	2 6 10 14





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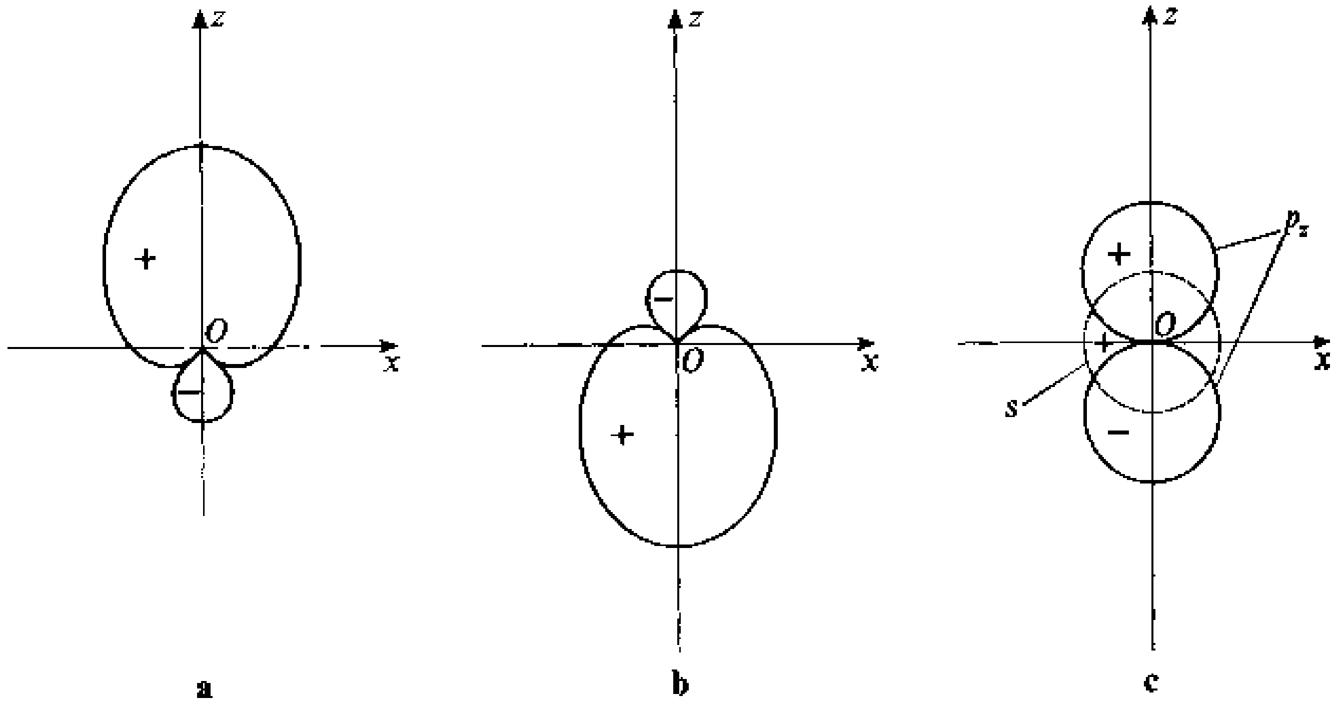
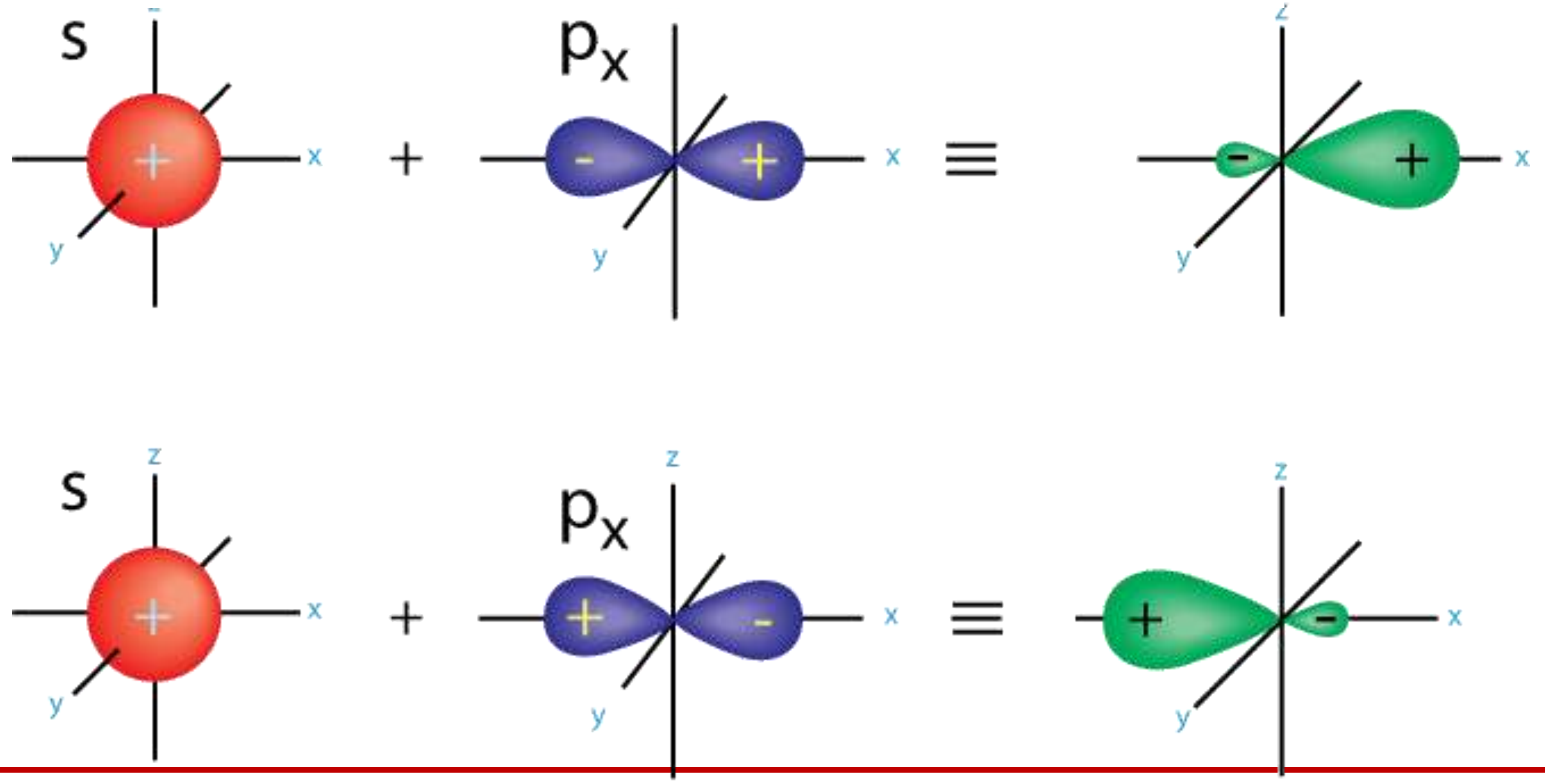
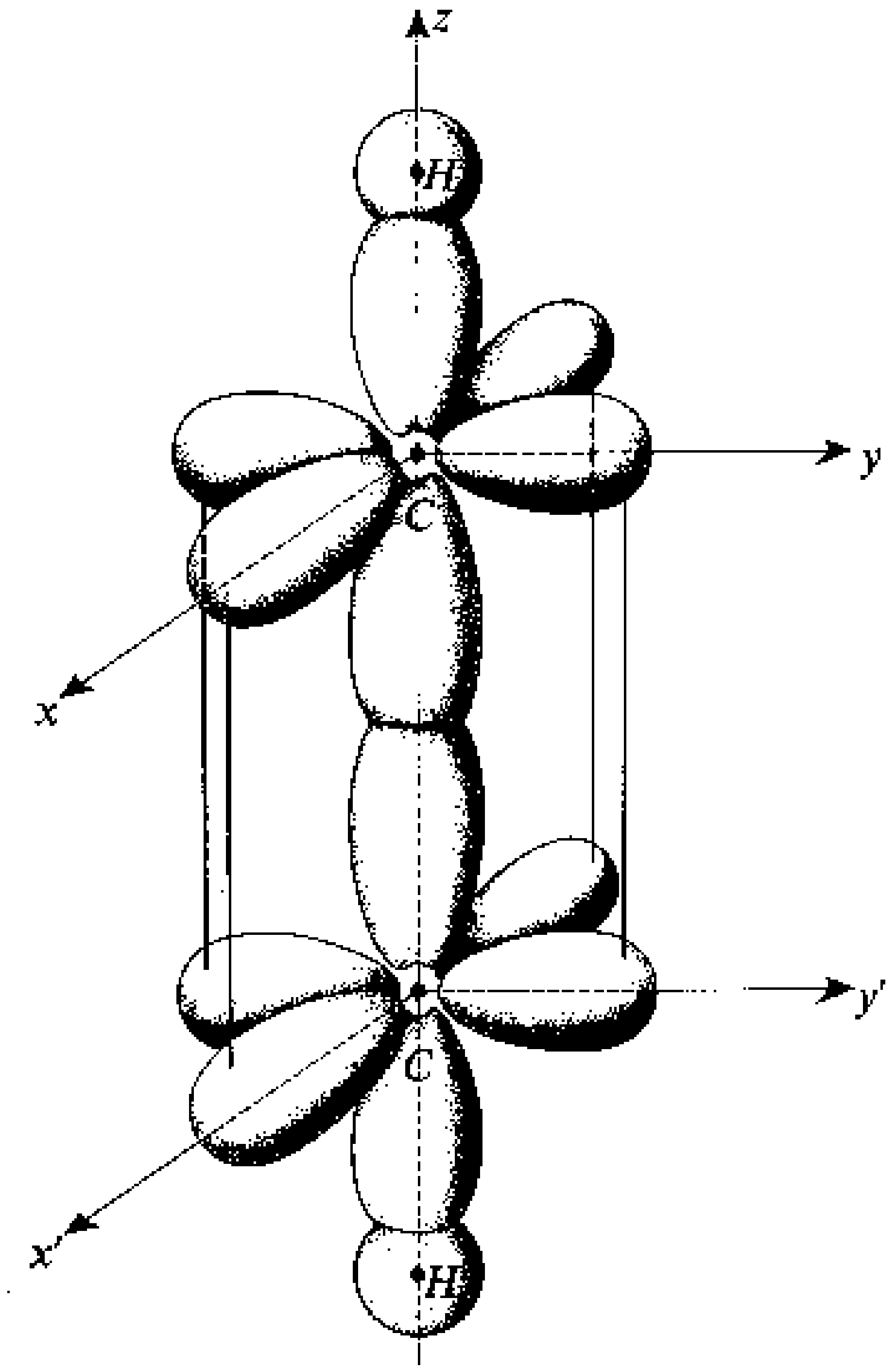
Covalent bond : *sp* hybridization





acetylene



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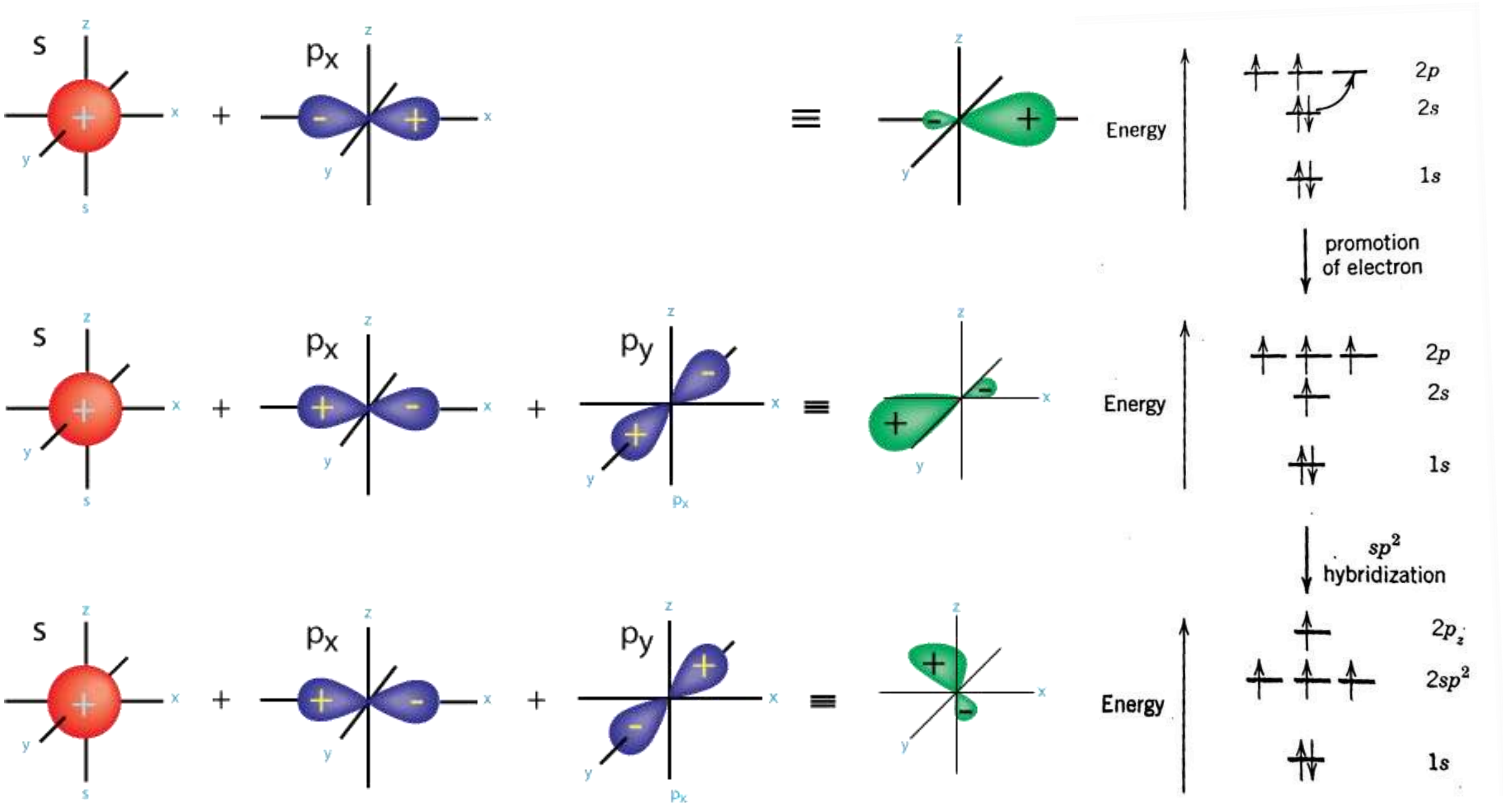
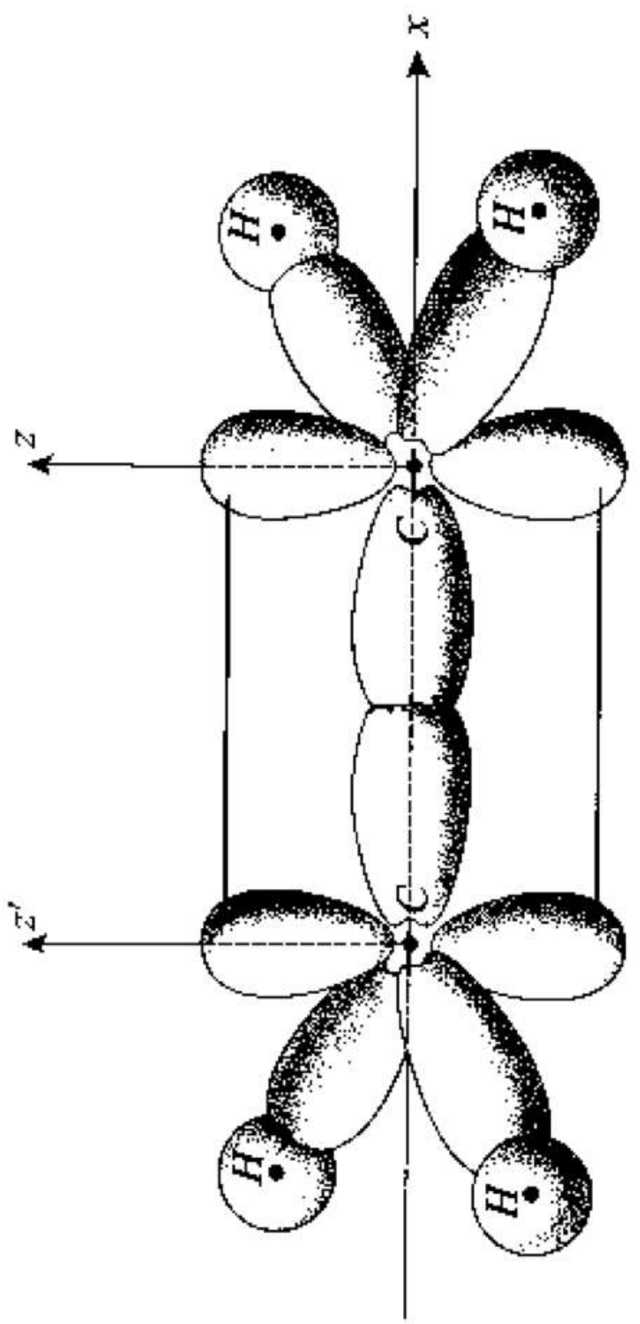
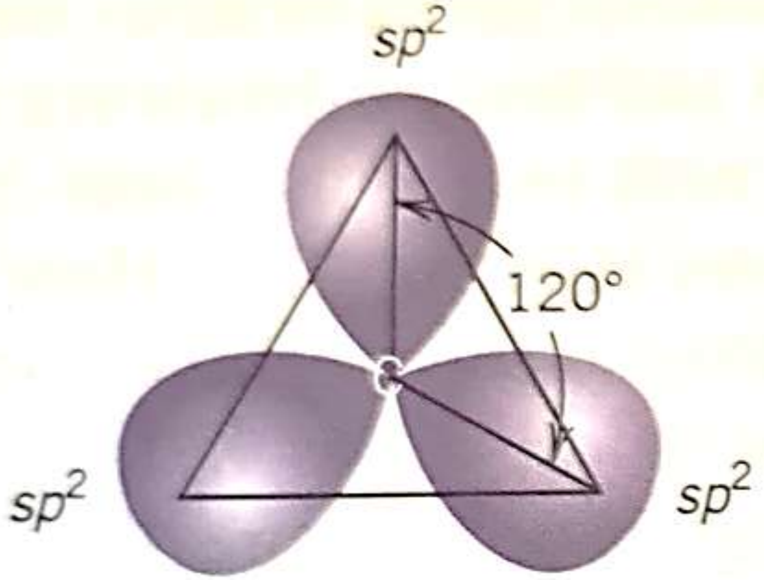
Covalent bond: *sp2* hybridization

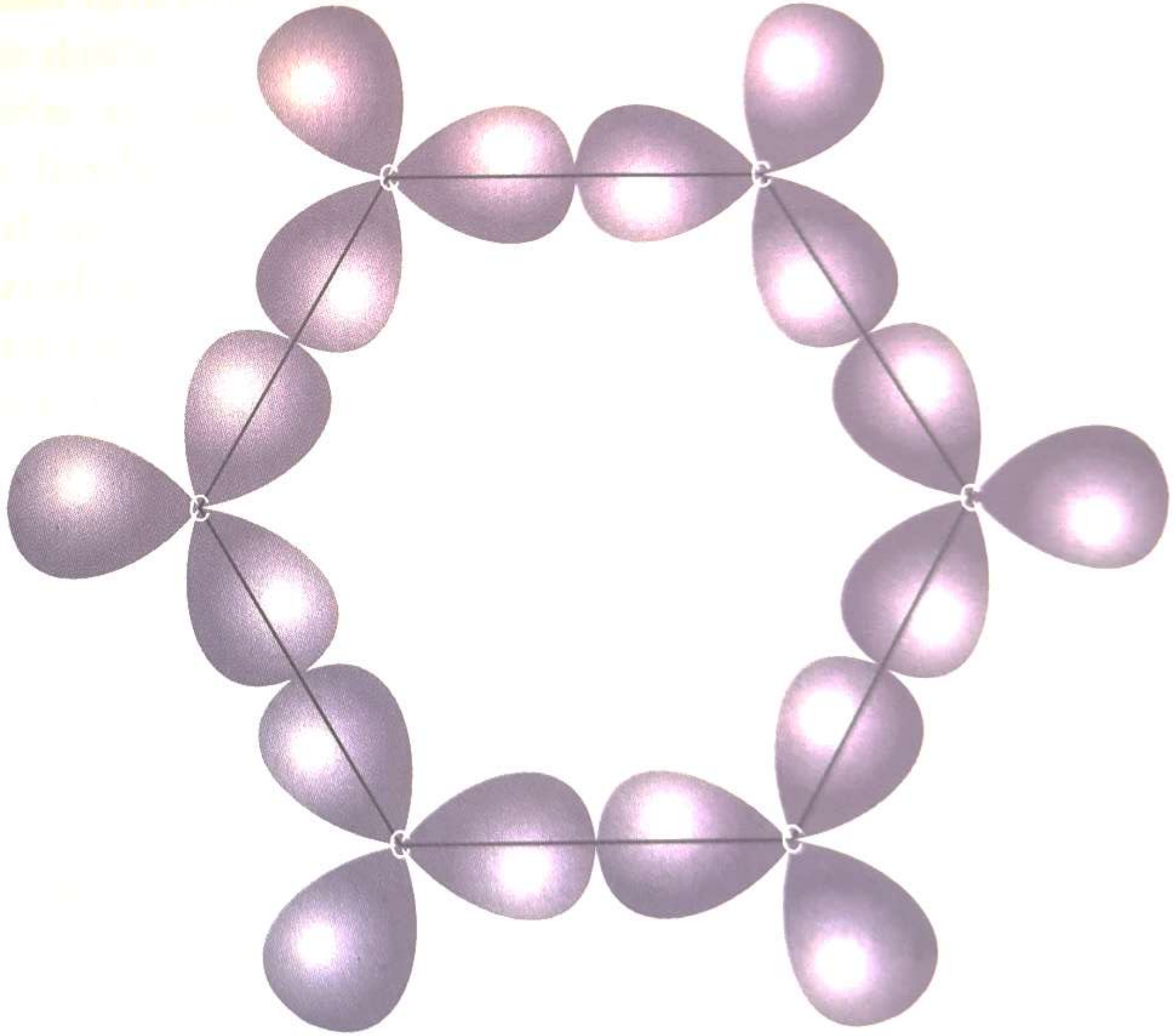


ethylene

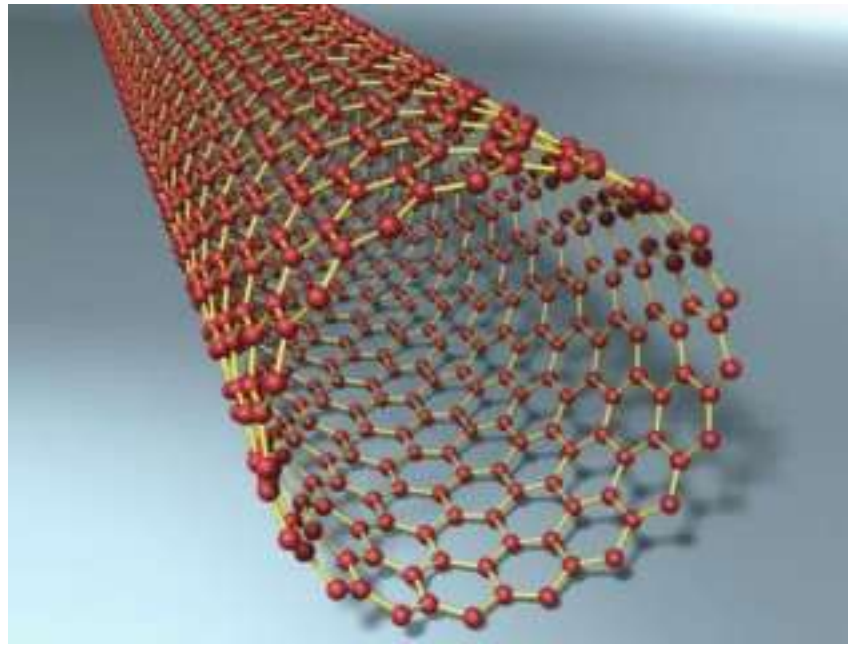


Covalent bond: *sp2* hybridization Graphite



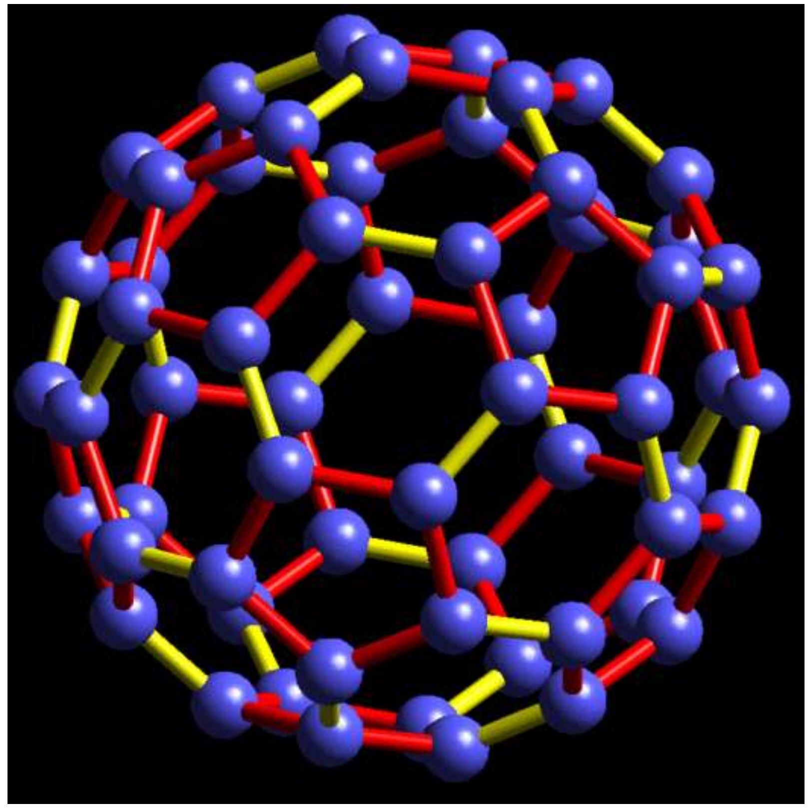


Covalent bond: examples



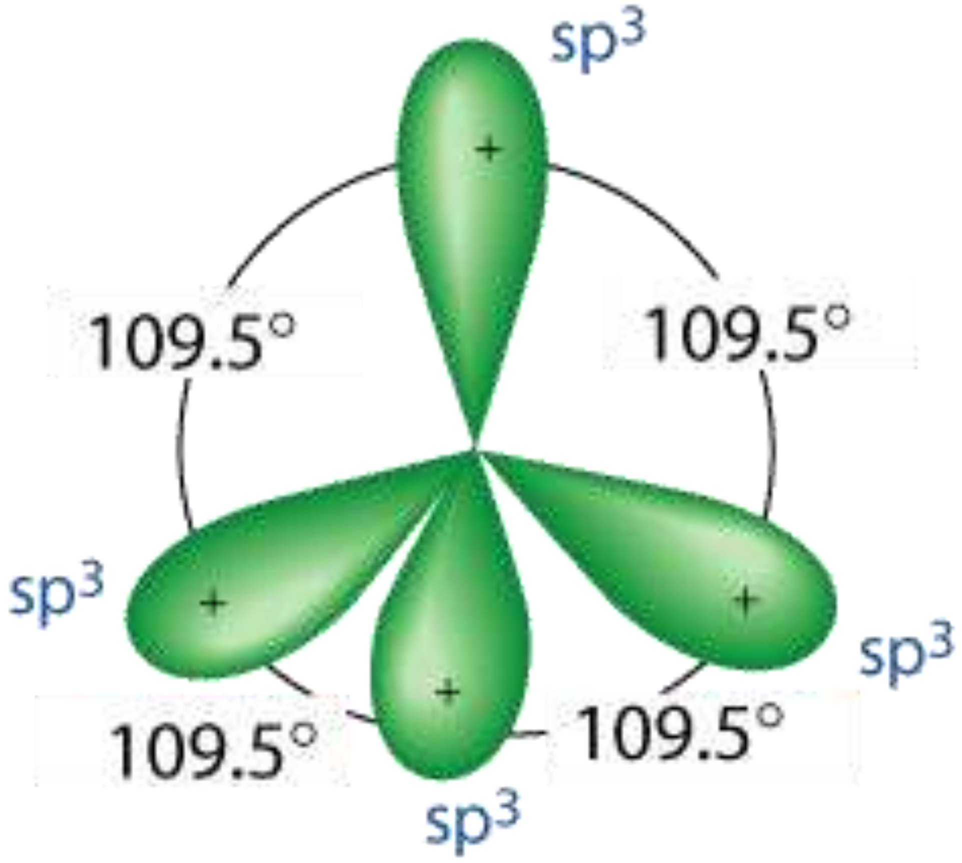
Carbon nanotube

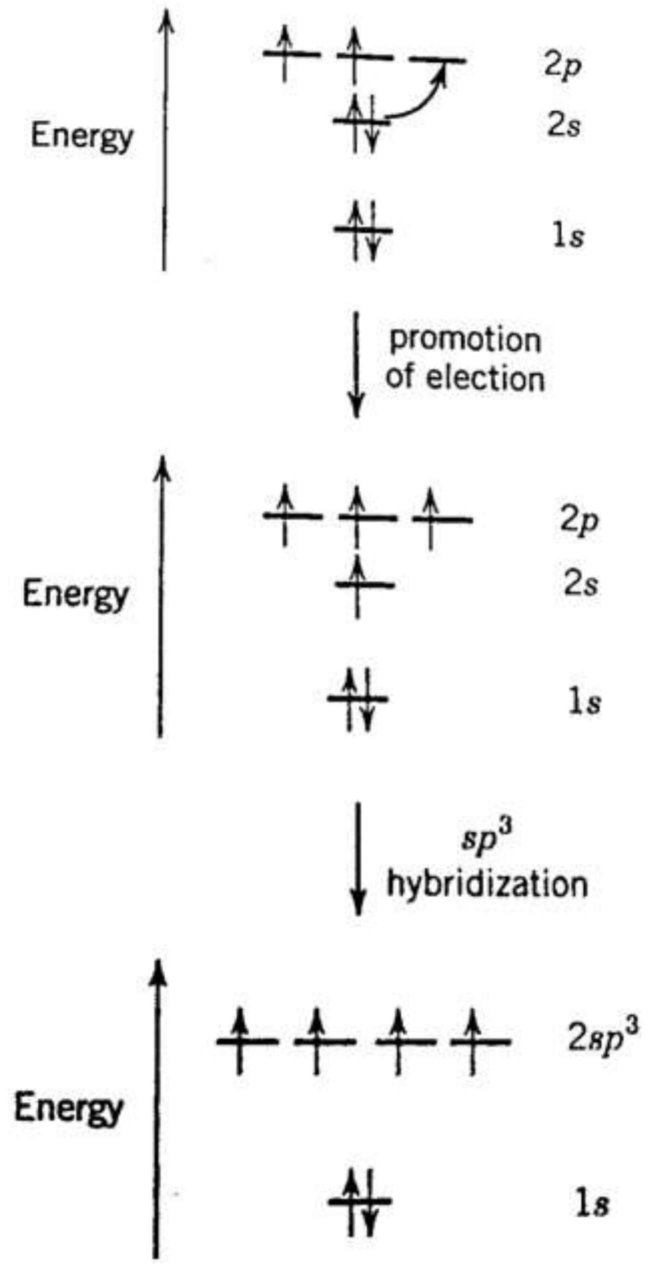
sp^2

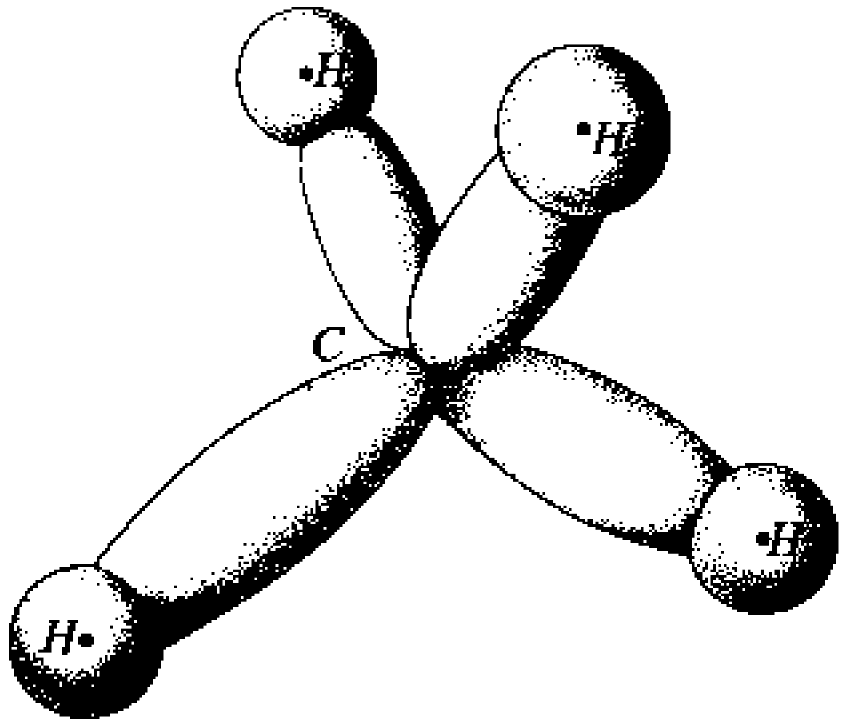


Bucky balls

Covalent bond: *sp3* hybridization

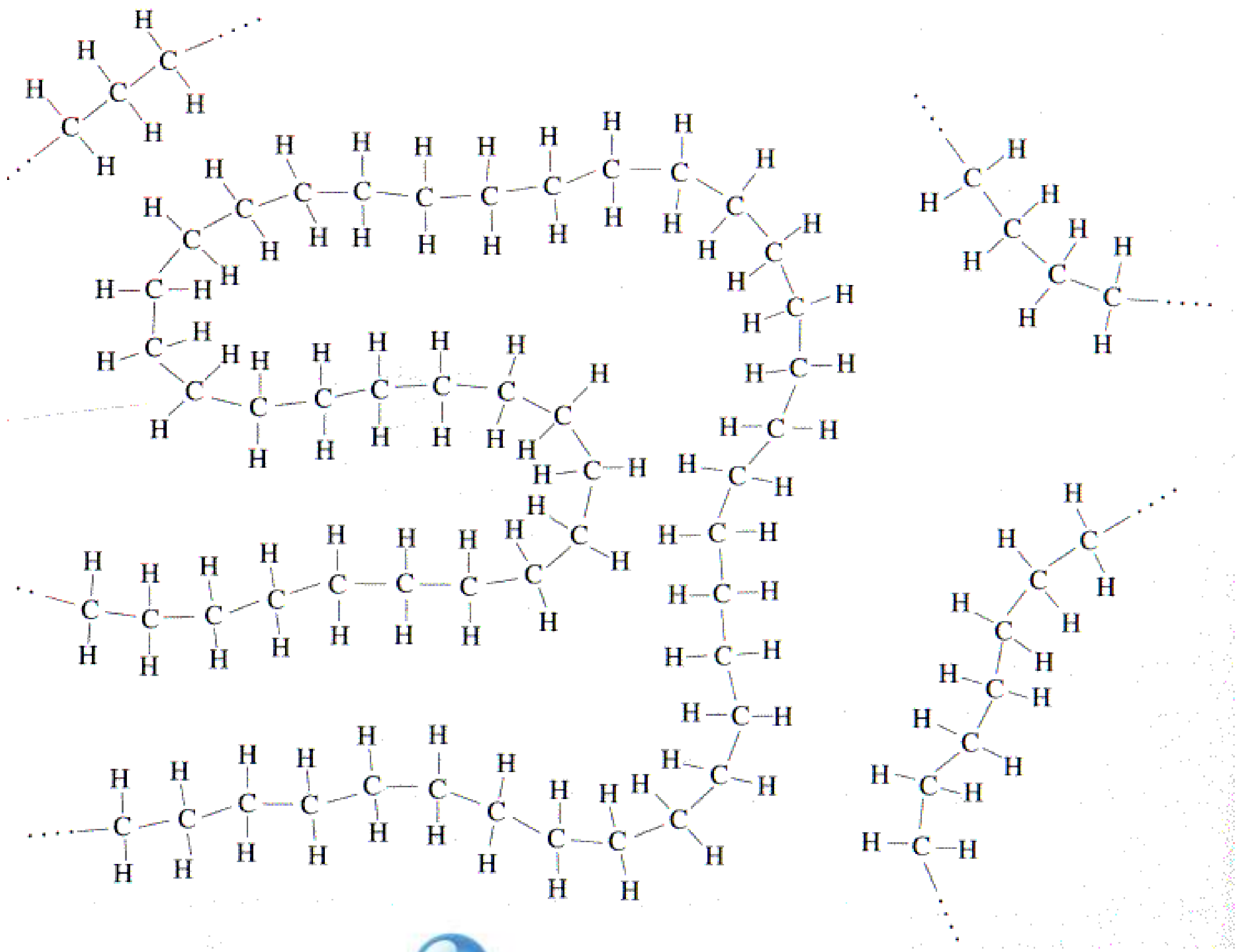






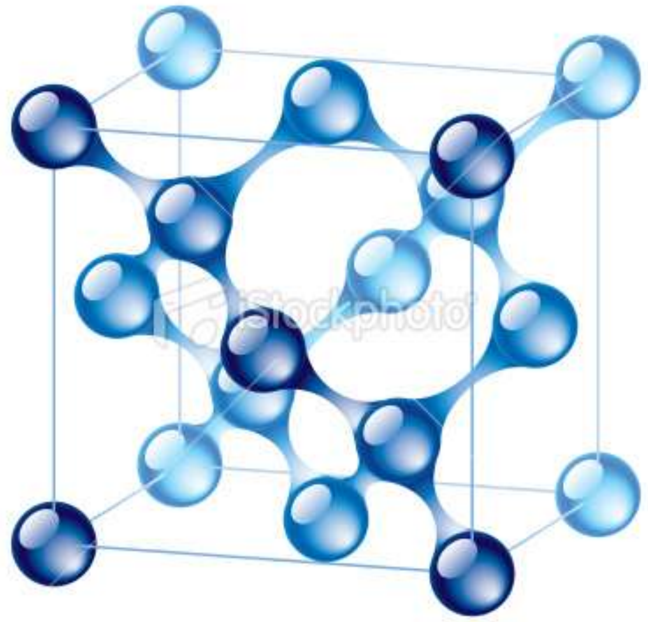
Methane

Covalent bond: examples



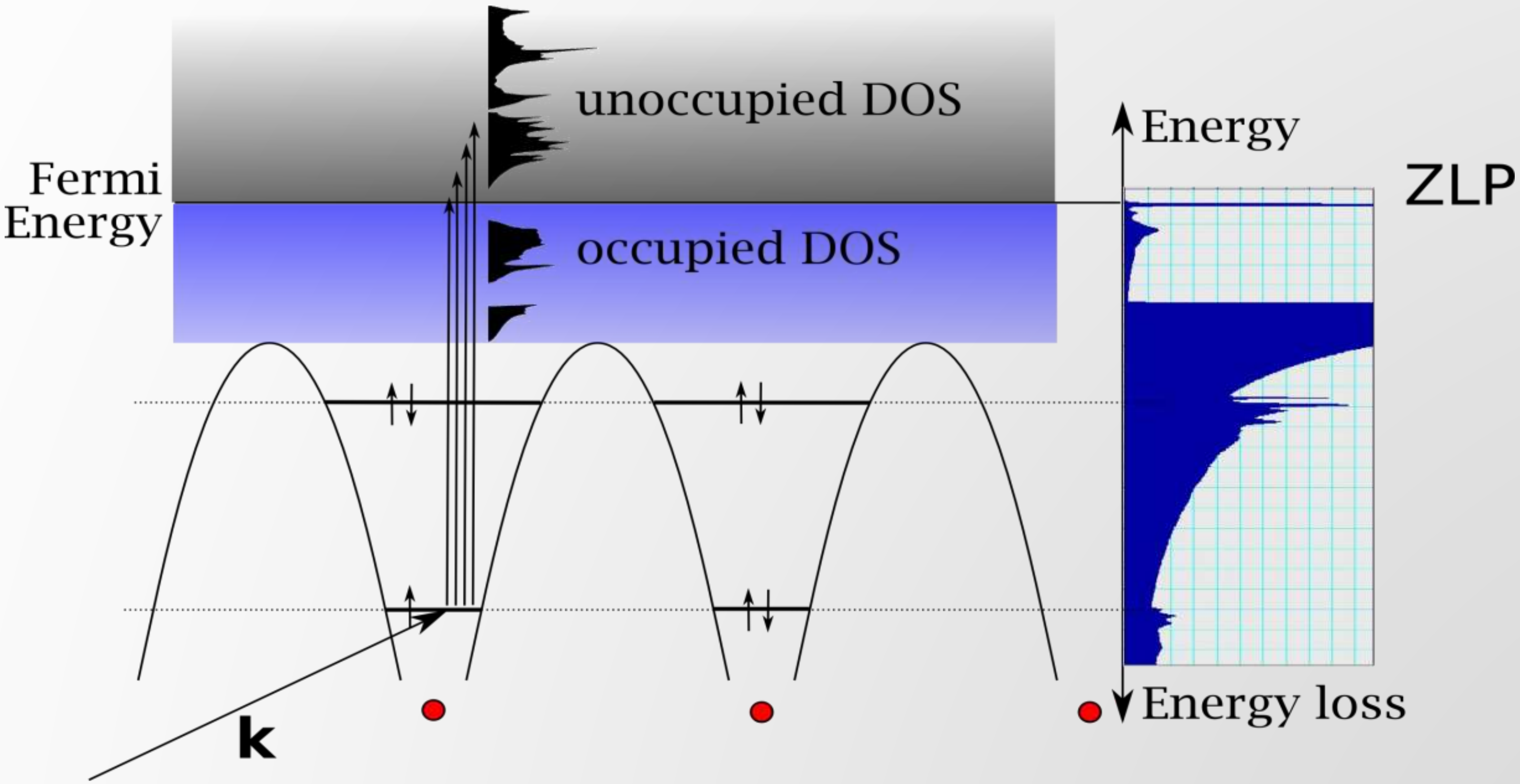
Poly-ethylene

sp^3



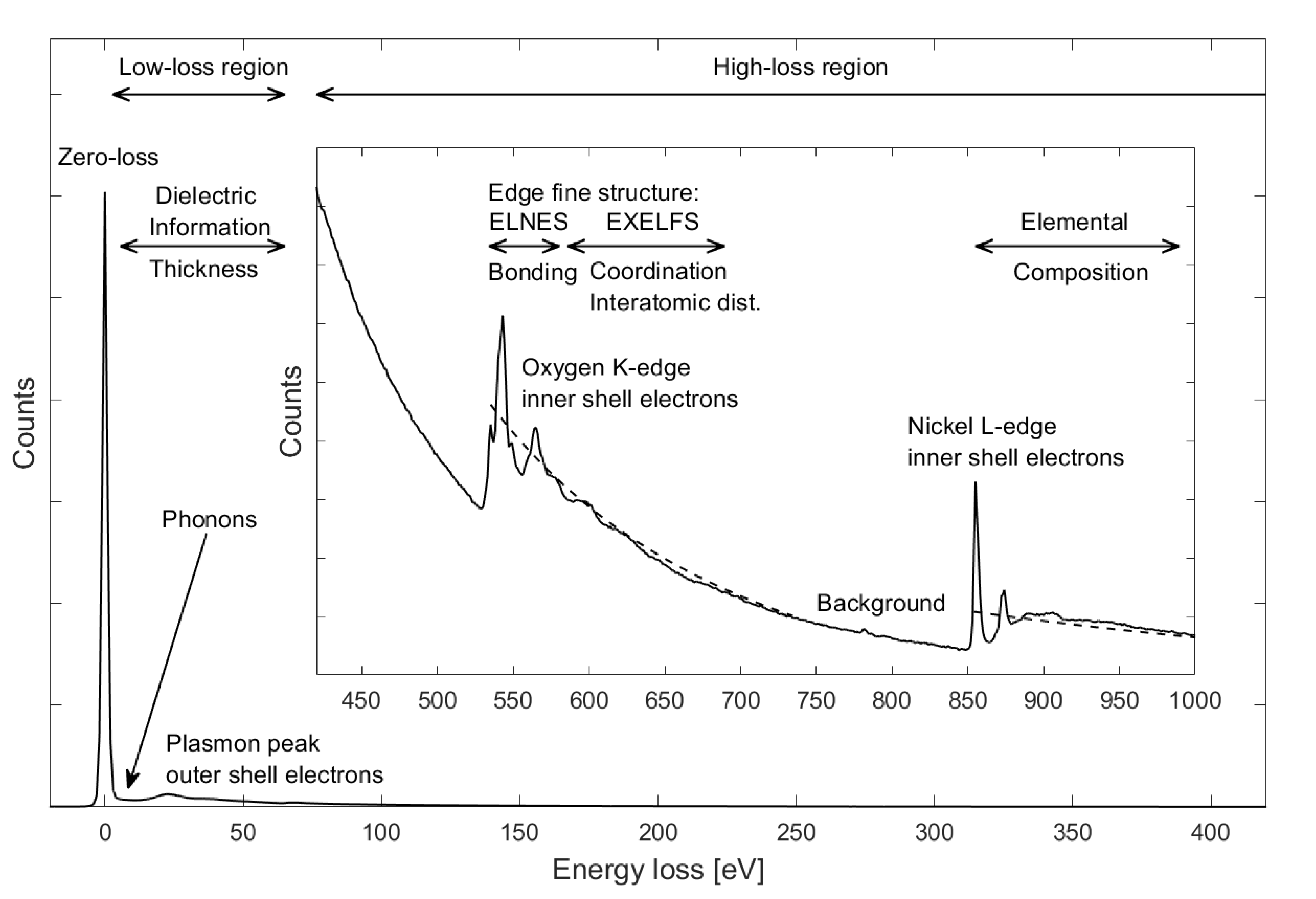
diamond sp^3

Electron Energy Loss Spectroscopy (EELS)



Core electron transitions from a localized core state to an unoccupied state. An onset energy is needed to reach the Fermi level, and transitions above the onset energy are possible.

Electron Energy Loss Spectroscopy (EELS)



<u>Low loss spectrum: plasmon and interband transitions</u>

- Optical properties
- Band gap (semiconductors
- Angular resolved: plasmon dispersions
- <1eV: phonons – vibrational spectroscopy

<u>High Loss spectrum:</u>

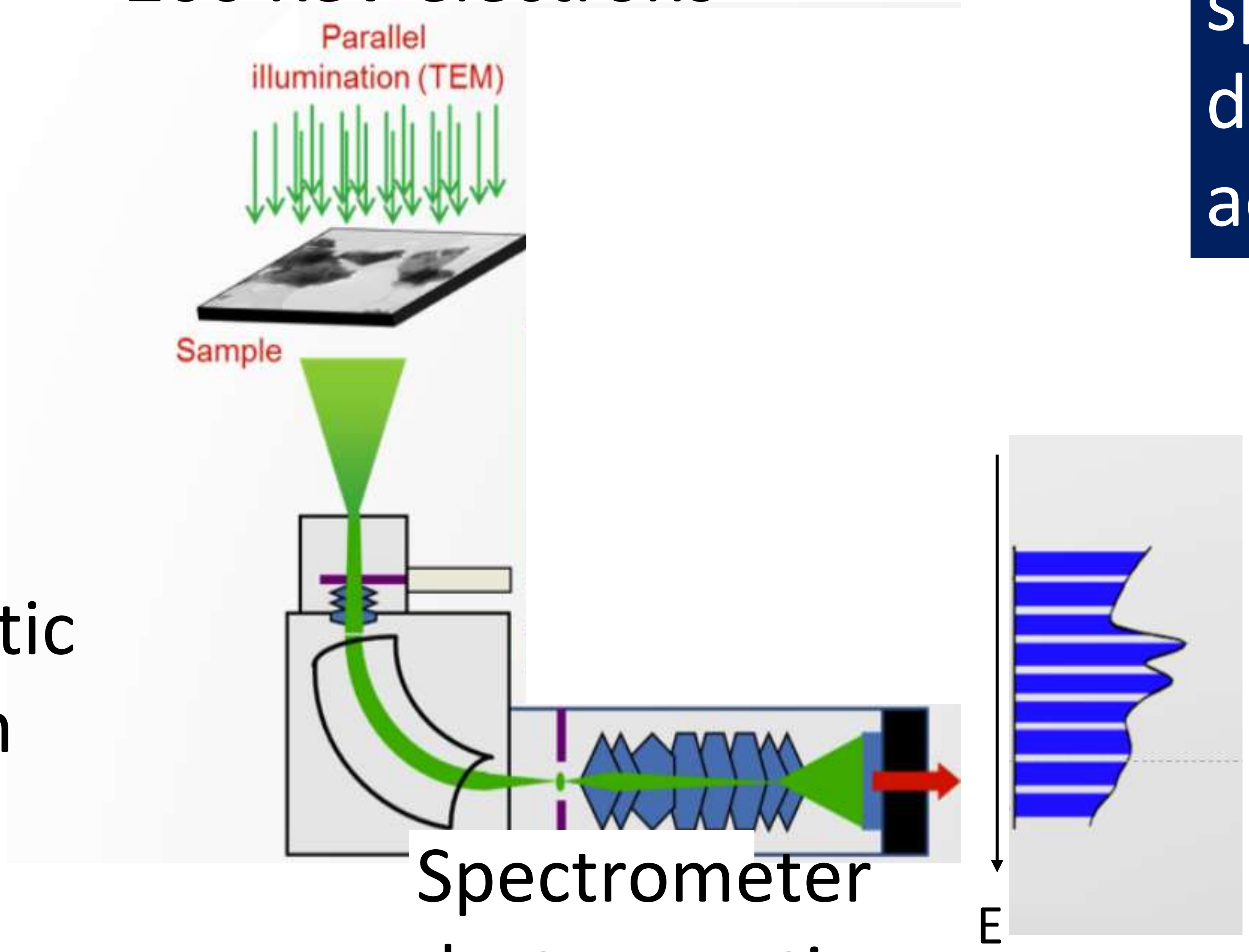
- Chemical composition
- Electronic structure (DOS)
- Magnetic properties- angle resolved core loss
- Nearest neighbor bonding correlations

Electron Energy Loss Spectroscopy (EELS)

Parallel illumination (TEM)
200 KeV electrons

The post-column electron spectrometer in the TEM disperses the electrons according to their energy.

Magnetic prism



Spectra captured on CMOS/CCD detector

Spectrometer electron optics

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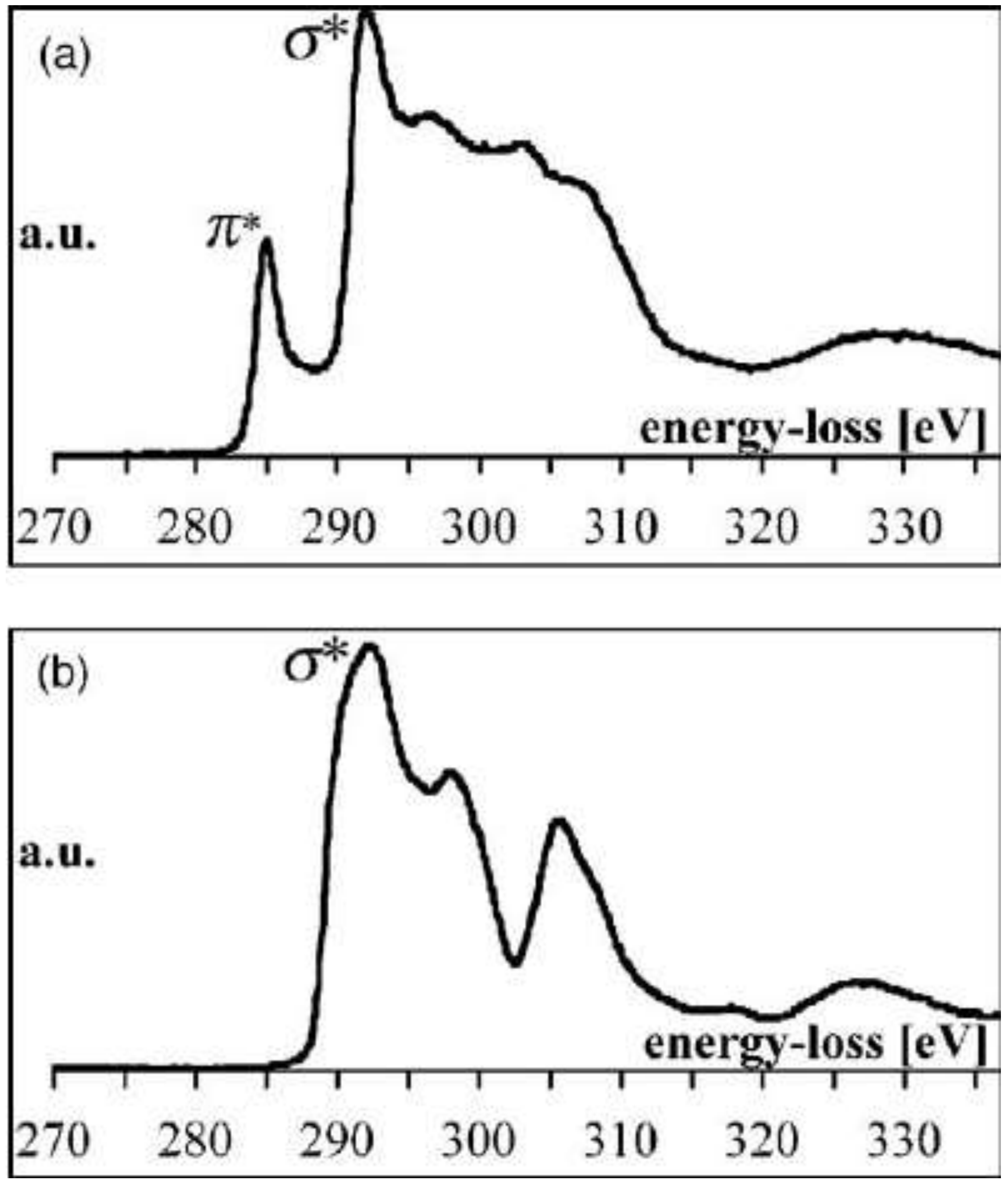
Covalent bond: EELS



Graphite sp^2

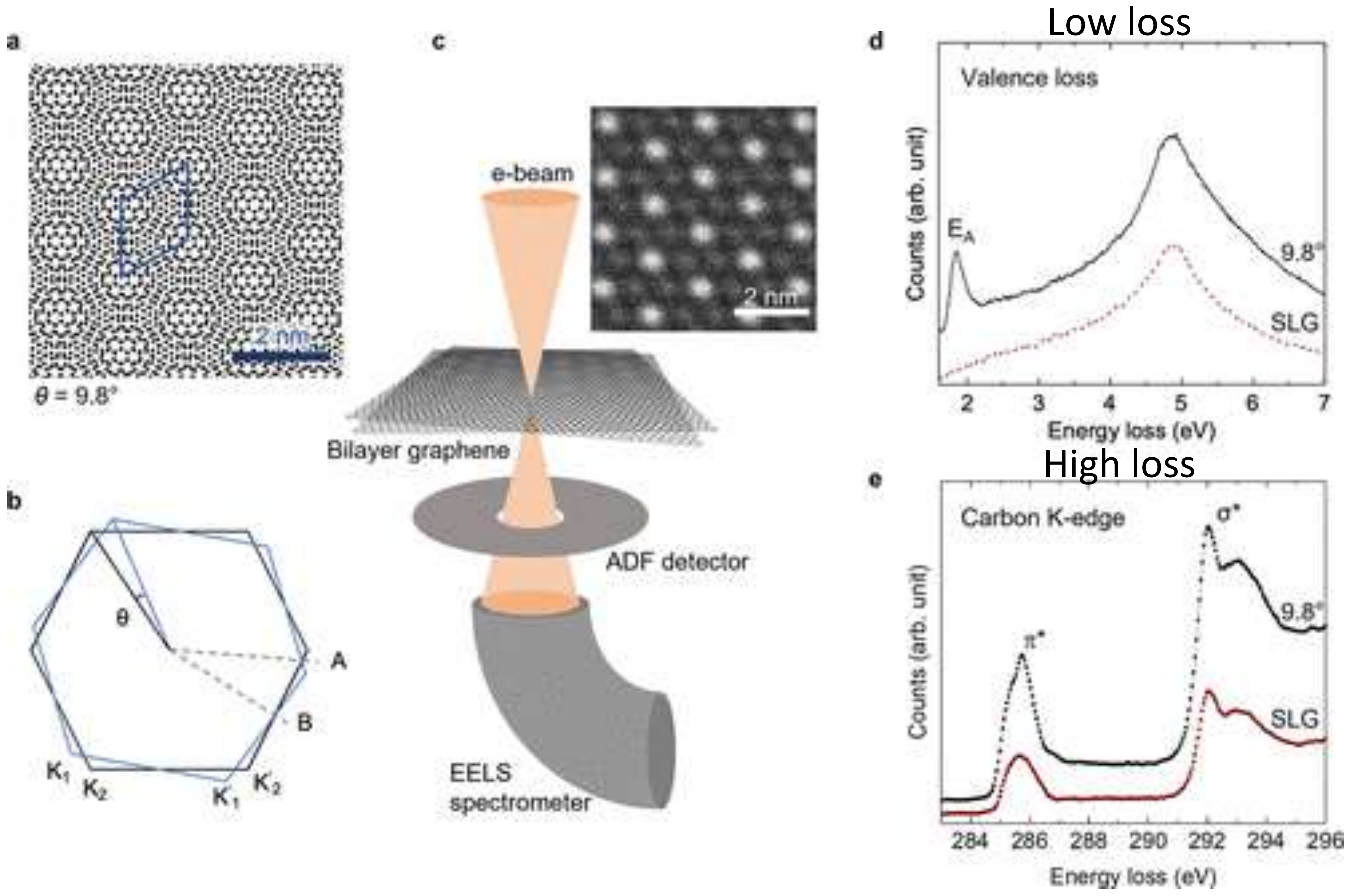
1 π bonds
3 σ bonds

Diamond sp^3

No π bonds
4 σ bonds

Electron Energy Loss Spectroscopy can measure the bond energy and ratios of π and σ bonds on ionization edges

EELS of twisted graphene bilayers



E_a peak observed in twisted bilayer

2x the counts observed in the bilayer as expected

Only Low loss Spectrum shows difference between single layer graphene (SLG) and 9.8 degree twisted bilayer graphene

Exercise: DEMO on EELS Today!

Chemistry Building CH H0 604

2 groups of 6-7 people

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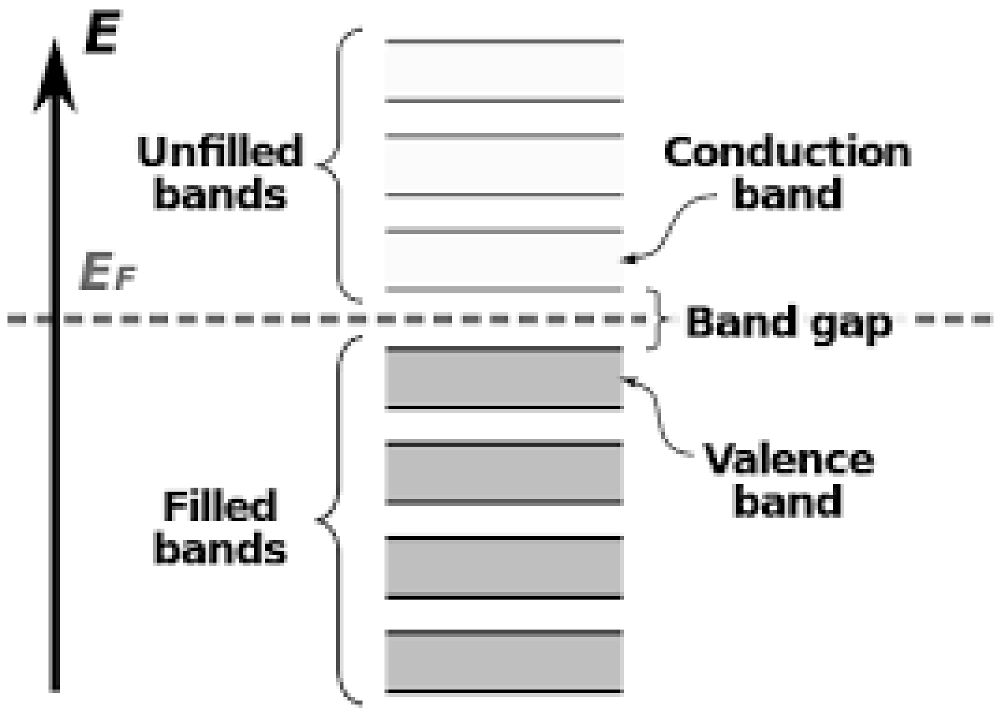
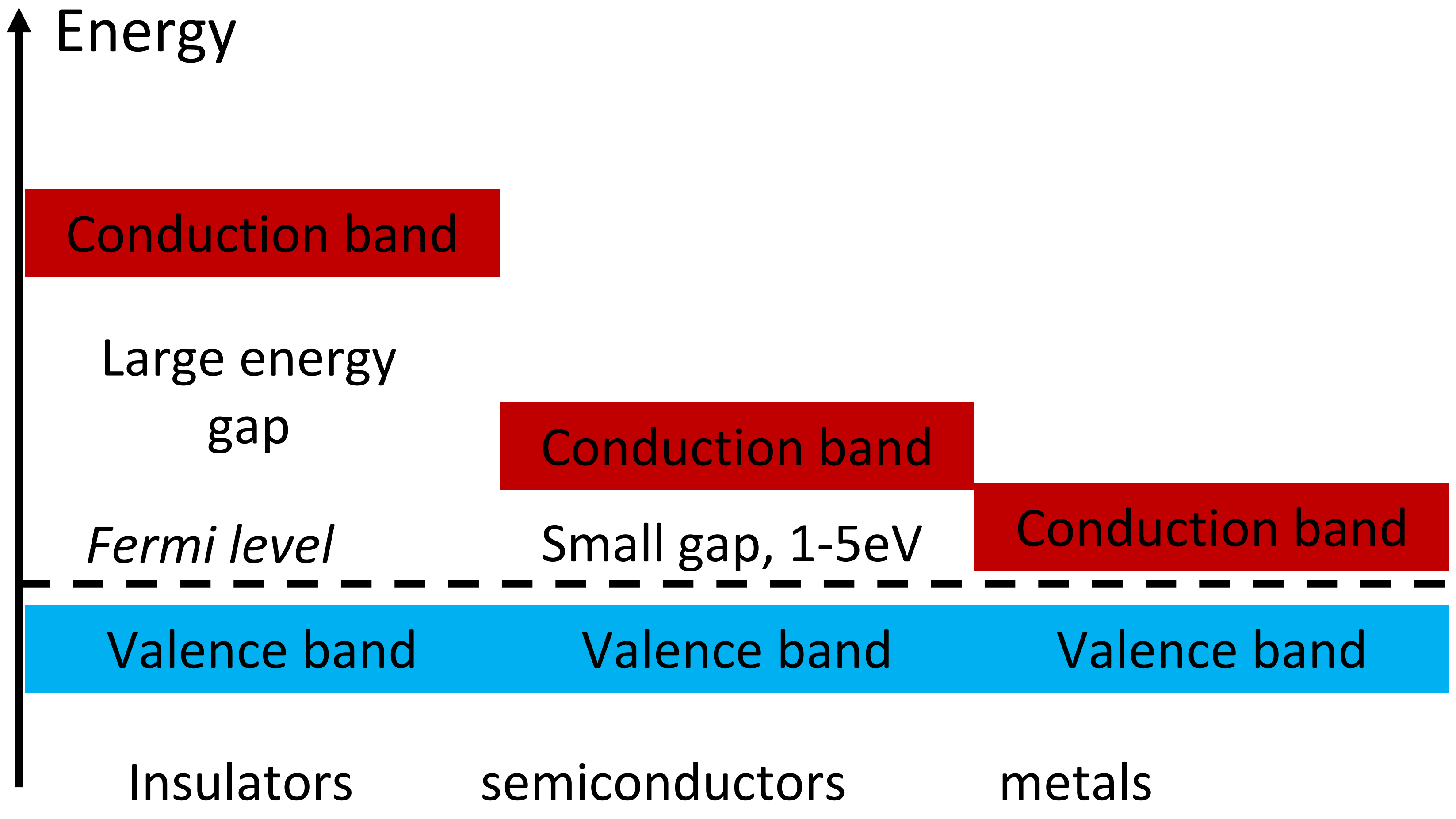
Metallic bonds

Metal bands





Metals have incomplete bands

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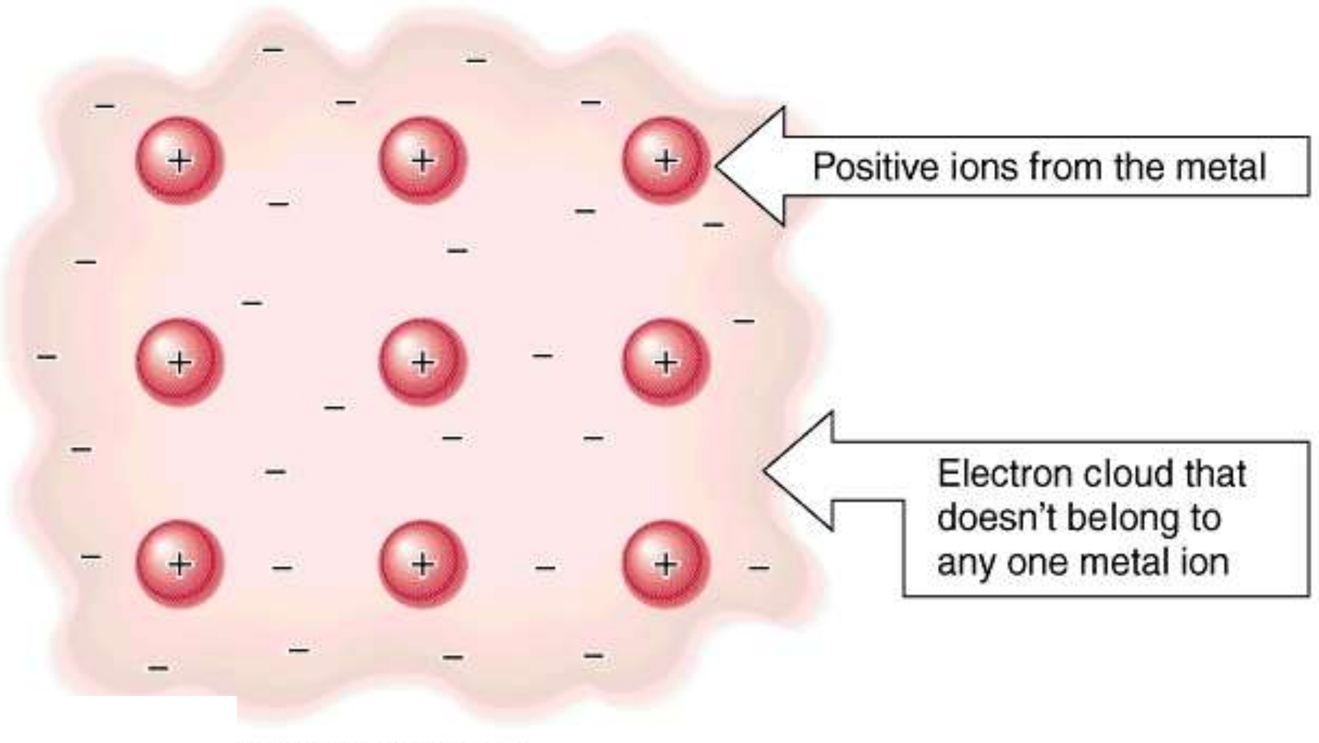
Metallic bond

- Metal bonds have available states (incomplete valance band) with wave vector k.
- The momentum of the electrons can be changed.
- Electrons in metal bonds have a net velocity component along the electric field directions, i.e., why metals are good conductors.



$$\psi_k(x) = u_k(x)e^{ikx}$$

Bloch wave functions

$$\psi_k(x+L) = \psi_k(x)$$

Boundary conditions of the L-size of the crystal

$$\psi(x) = \sum_k C(k)e^{ikx}$$

Fourier decomposition

Wave equation in a periodic potential

$$U(x) = U(x+a)$$ $U(x)$ is real

Fourier (periodic potential) $$U(x) = \sum_G U_G e^{iGx} \qquad U(x) = \sum_{G>0} U_G (e^{iGx} + e^{-iGx}) = 2\sum_{G>0} U_G \cos Gx$$

$$(H_0 + H_1)\cdot\psi = (E_0 + \Delta E)\cdot\psi \qquad \left(\frac{1}{2m}p^2 + U(x)\right)\psi(x) = \left(\frac{1}{2m}p^2 + \sum_G U_G e^{iGx}\right)\psi(x) = E\psi(x)$$

Fourier (wave function) $$\psi(x) = \sum_k C(k) e^{ikx}$$

Time-independent Schrödinger equation

Kinetic energy $$\frac{1}{2m}p^2\psi(x) = \frac{1}{2m}\left(-i\hbar\frac{d}{dx}\right)^2\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = \frac{\hbar^2}{2m}\sum_k k^2 C(k) e^{ikx}$$

Potential energy $$\left(\sum_G U_G e^{iGx}\right)\psi(x) = \sum_G\sum_k U_G e^{iGx} C(k) e^{ikx}$$

Central equation

Eigenvalue Solution to Schrödinger's equation

$$(\lambda_k - E)C(k) + \sum_G U_G C(k-G) = 0 \qquad C(k)?$$

Lets suppose $\quad U_G = U_{-G} = U$ and $U_{\pm nG} = 0 \quad n > 1$

$$U(x) = Ue^{ikx} + Ue^{-ikx} = 2U\cos(kx)$$

$$\lambda_k = \hbar^2 k^2 / 2m$$

$$\begin{vmatrix} \lambda_{k-2G} - E & U & 0 & 0 & 0 \\ U & \lambda_{k-G} - E & U & 0 & 0 \\ 0 & U & \lambda_k - E & U & 0 \\ 0 & 0 & U & \lambda_{k+G} - E & U \\ 0 & 0 & 0 & U & \lambda_{k-2G} - E \end{vmatrix} = 0$$

$$\uparrow \qquad \uparrow \qquad \uparrow \qquad \uparrow \qquad \uparrow$$

$$C(k-2G) \quad C(k-G) \quad C(k) \quad C(k+G) \quad C(k+2G)$$

solutions

$$E(k)$$

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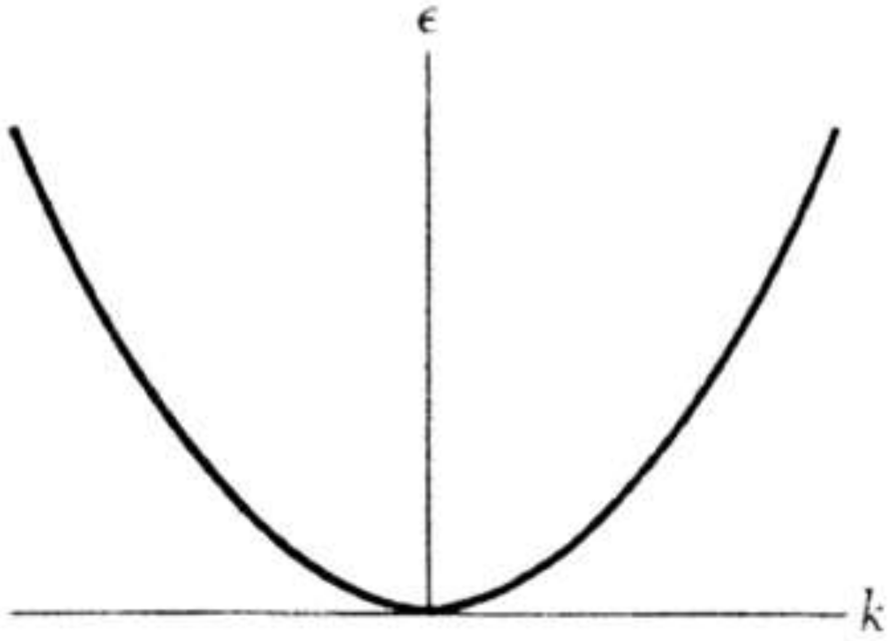
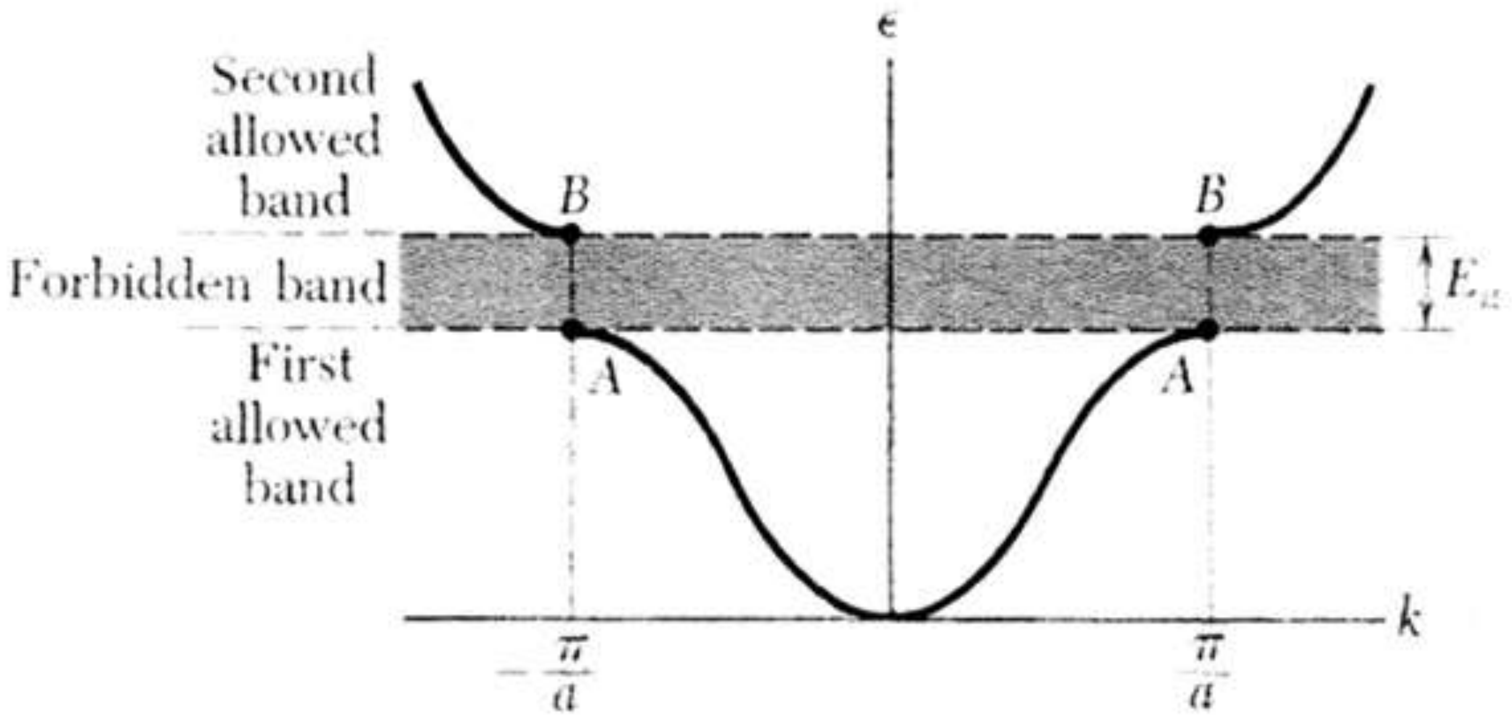
Nearly Free Electron (NFE) model

In the absence of the periodic potential t, electrons would behave as free particles with plane-wave states and a quadratic dispersion relation

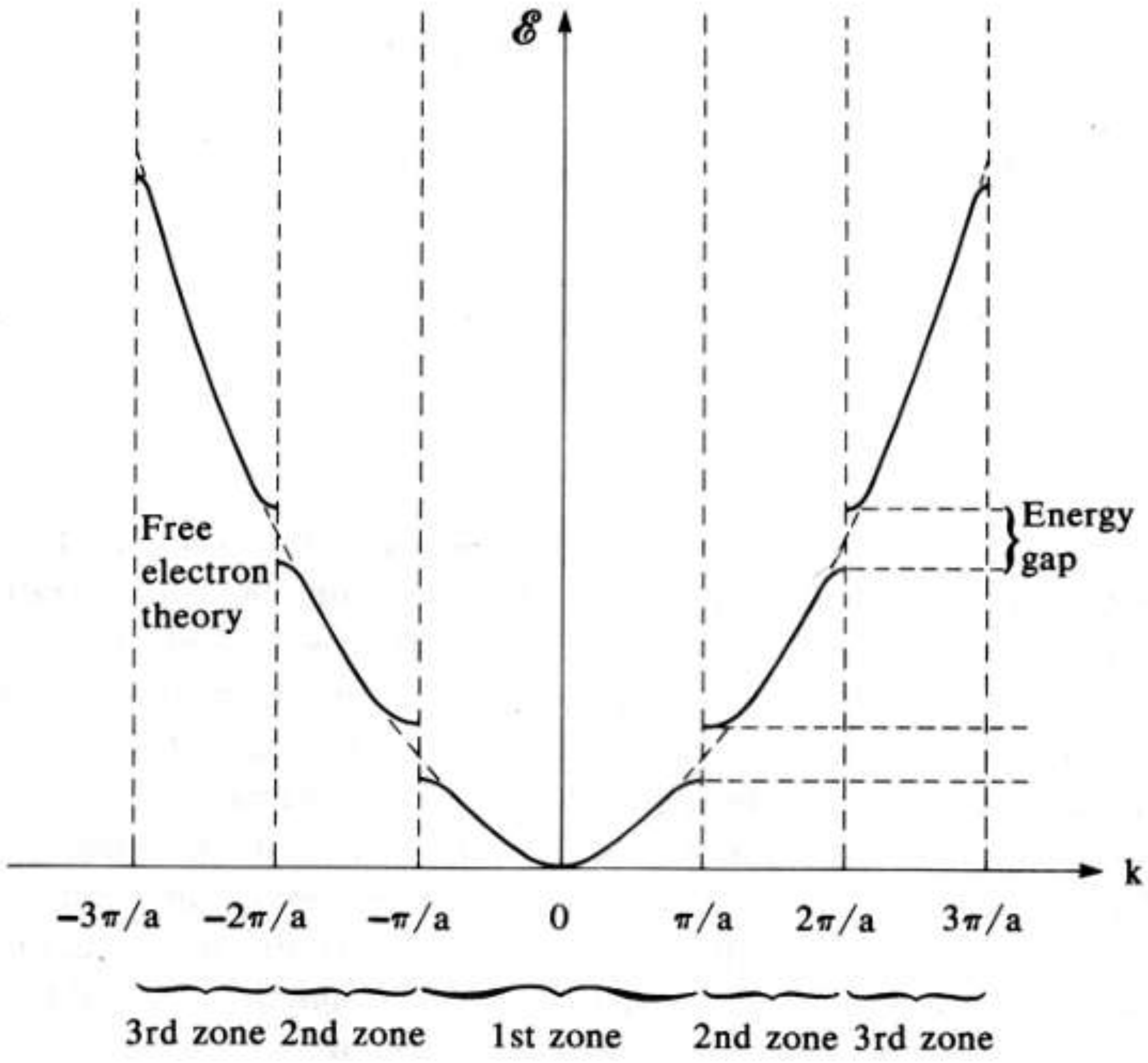
$$E(k) = \hbar^2 \vec{k}^2/2\,m, \;\; \vec{k}^2 = (k_x^2 + k_y^2 + k_z^2)$$

At these boundaries, wavevectors $\vec{k}$ and $\vec{k} + \vec{G}$ correspond to degenerate free-electron states, where $\vec{k} = \pm n\pi/L$. The periodic potential couples these degenerate states, and the resulting hybridization lifts the degeneracy and opens an energy gap





Nearly Free Electron (NFE) model



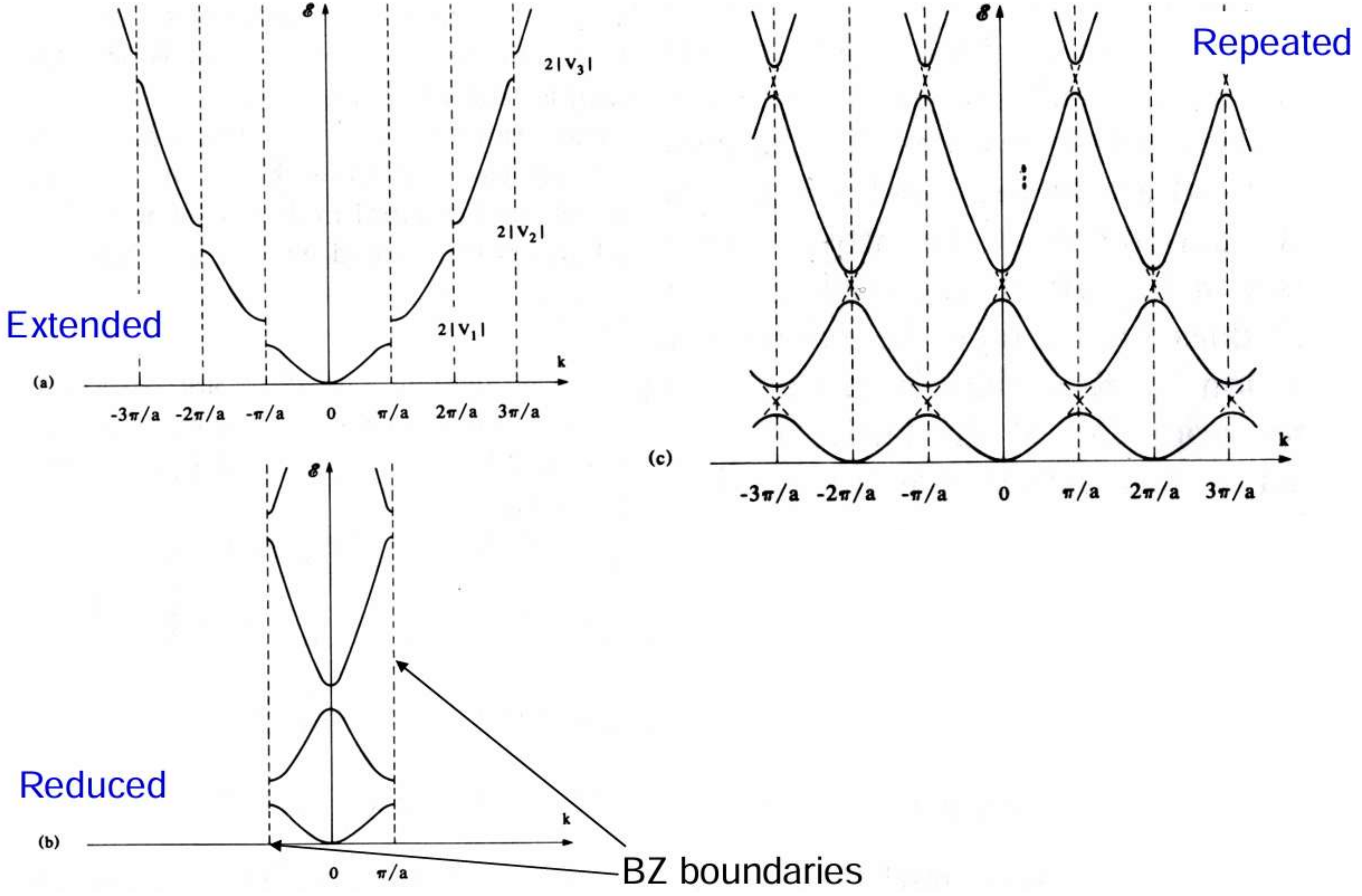
In periodic crystal structure and under the condition, $\vec{k} = \pm\vec{G}/2 = \pm n\pi/a$

The electron wave undergoes Bragg scattering and produces reflections.

Energy gaps develop at $\vec{k}$ due to these reflections. Note: at $\vec{k} = \pm\, \pm n\pi/a$, the wavefunctions are not traveling electrons waves.

The region between $-\frac{\pi}{a}$ $and\, \frac{\pi}{a}$ is the first **Brillouin zone** of this 1D lattice

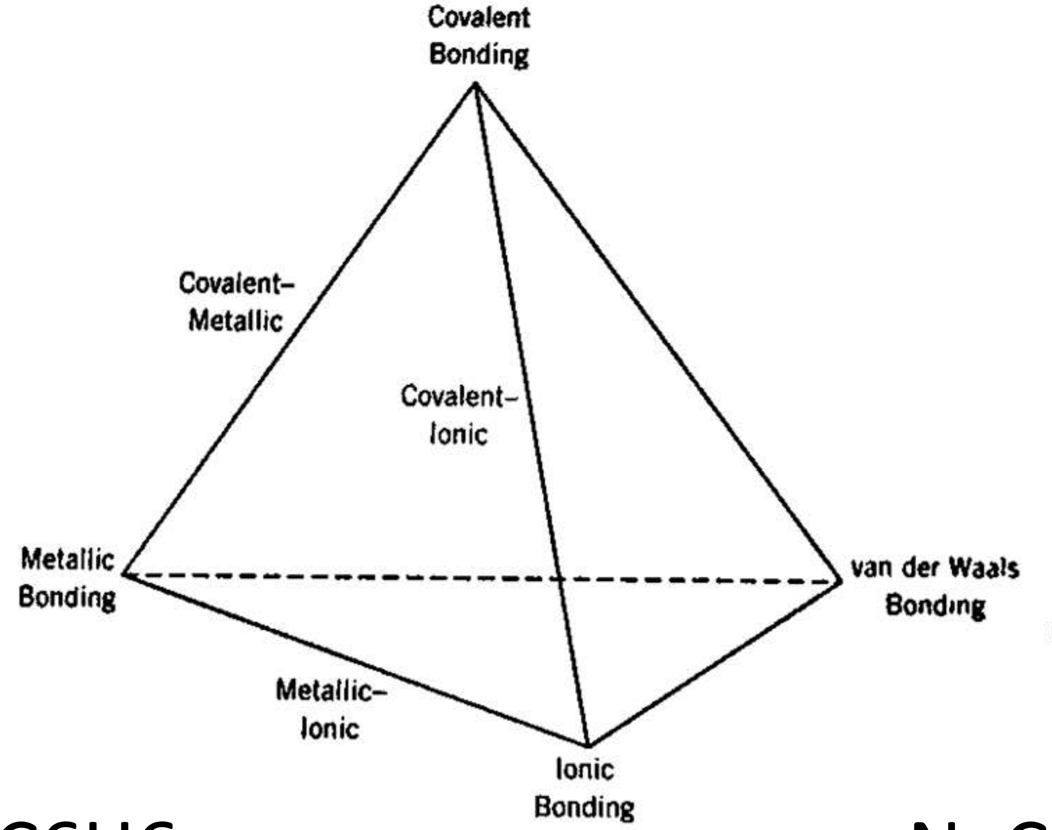
Nearly Free Electron (NFE) model

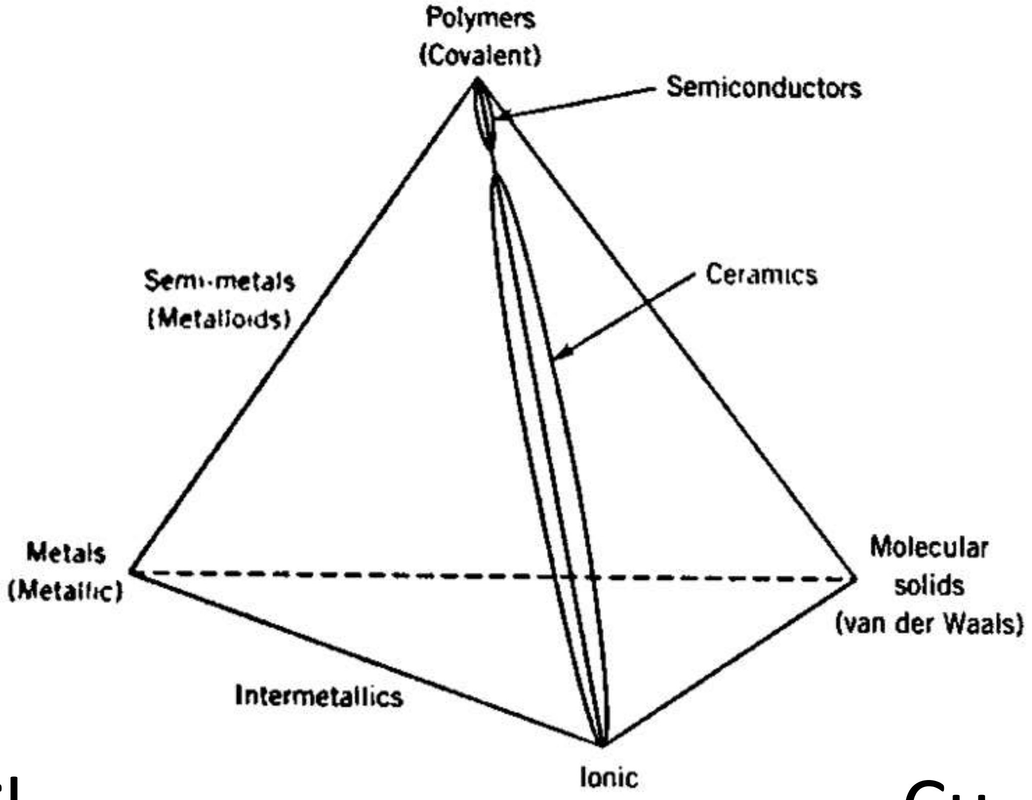


The magnitude of the band gaps depends on the strength of the periodic potential:

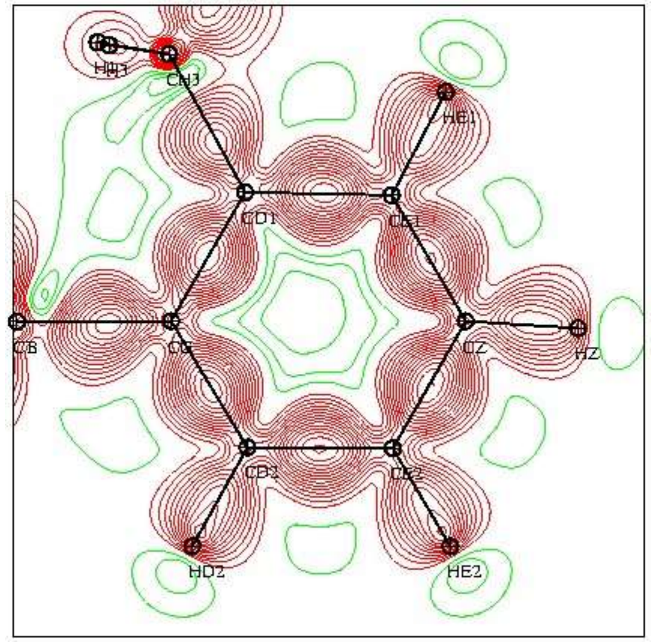
- in weak potentials, the gaps are small and the bands resemble those of a free electron gas
- in stronger potentials, the bands become more distorted, and the NFE model provides a stepping stone to the tight-binding picture.

Chemical bonds and materials

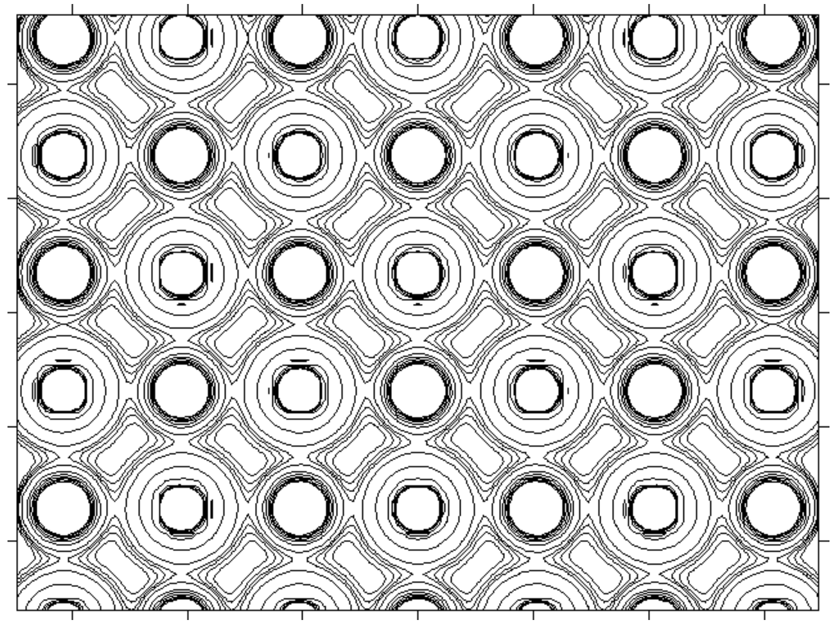




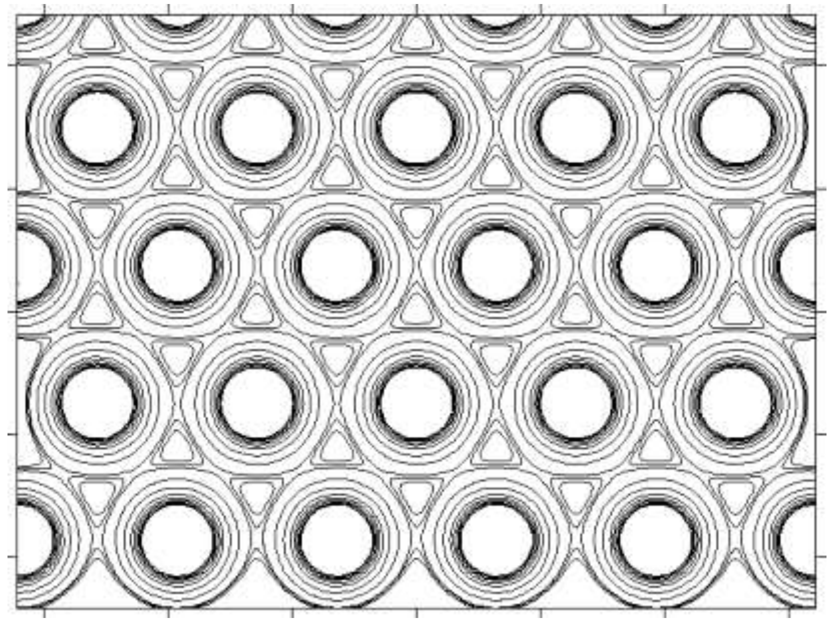
C6H6



NaCl



Cu



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