Atomic structure, interactions, AFM

Medical Biophysics I. 8 October, 2025.

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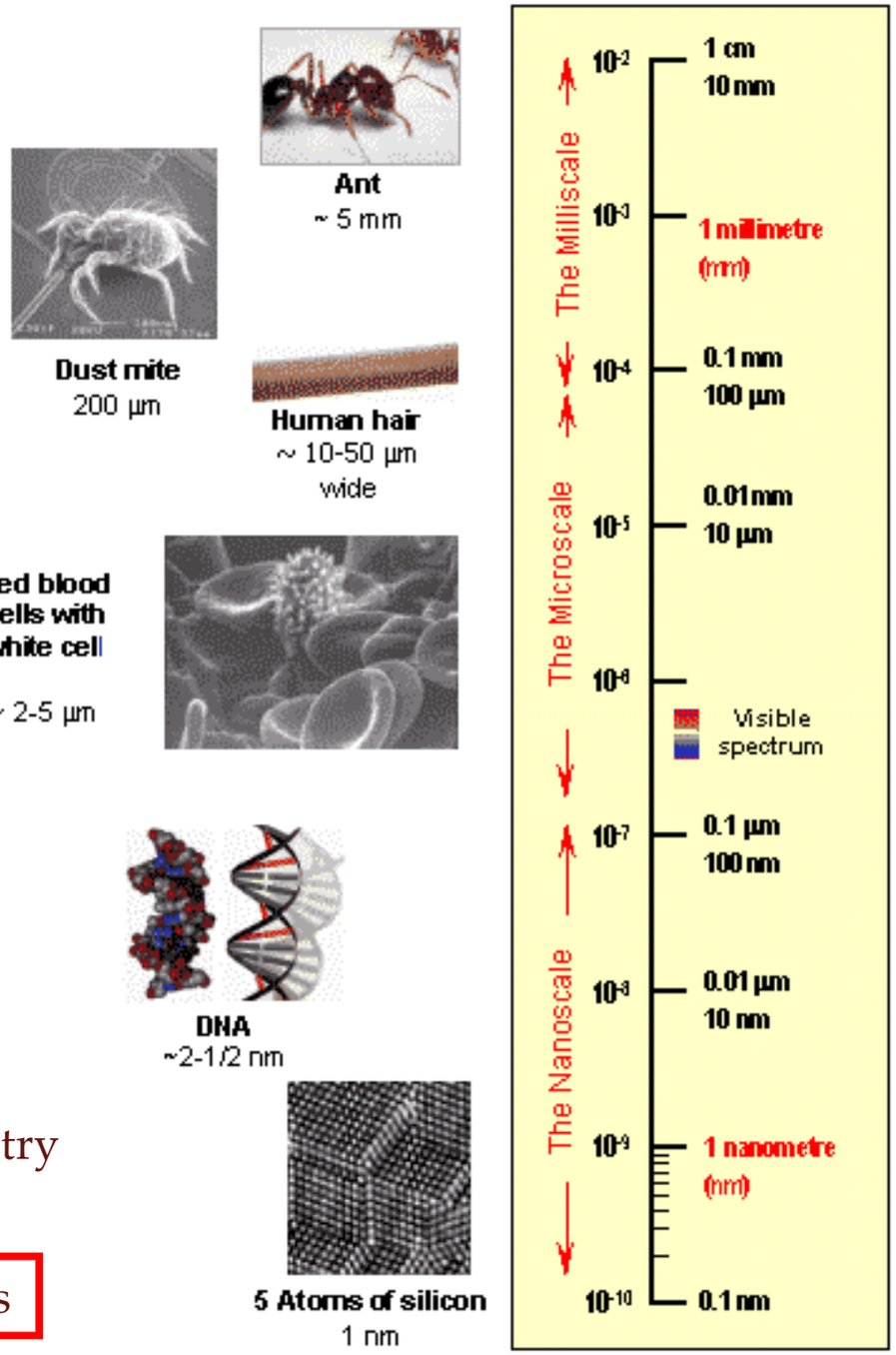
SEMMELWEIS EGYETEM 1769

Dimensions of Living Systems

Thermodynamics

10^{23} Atoms



Mesoscale

10^{10} Atoms

10^{3} Atoms

Quantum chemistry

10^{1} Atoms

Quantum physics

10^{0} Atom

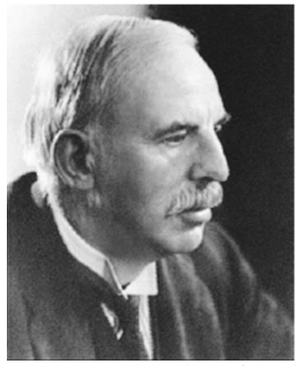
Richard P. Feynman (Nobel prize, 1965):

If, due to a disaster, the knowledge of humankind were destroyed, and only one sentence could be passed on to future generations, what would be the statement that best summarizes our knowledge? Atomic theory: The entire natural world is made up of particles that constantly move and attract or repel each other. The characteristics and processes of nature can be described through the atomic particles.

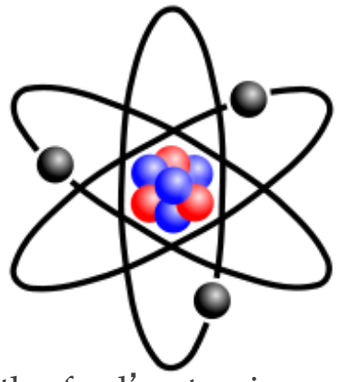
Early atomic models

Democritus (460-370 BC)
Matter composed undivisible particles (atomos).

Joseph John Thomson (1856-1940)
Discovery of the electron.

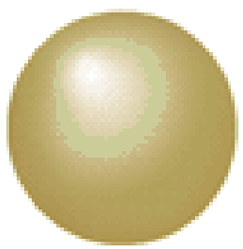


Ernest Rutherford
(1871-1937)



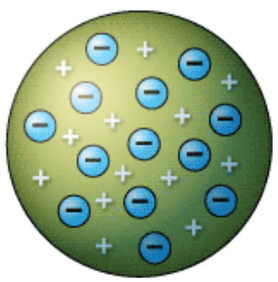
Rutherford's atomic model: miniature planetary system

John Dalton (1766-1844)
A given element composed of identical, undivisible atoms.



Dalton's atom

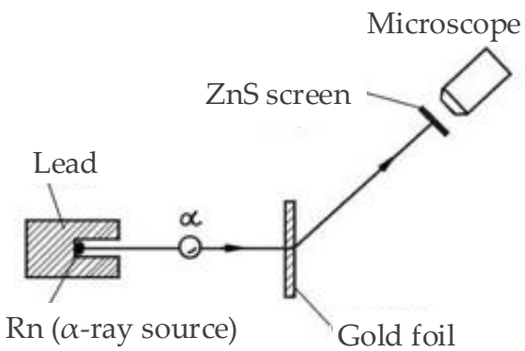
Cathode ray (electron beam) in vacuum tube.

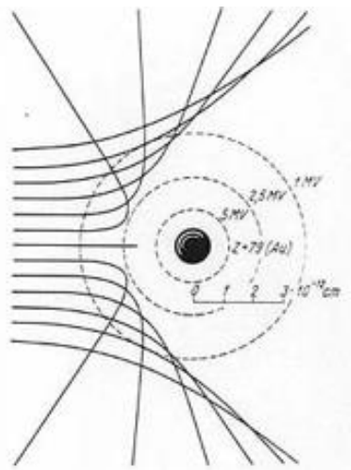


"Plum pudding" atomic model

Rutherford experiment

The diameter of the nucleus is 10,000-100,000 times smaller than that of the atom!





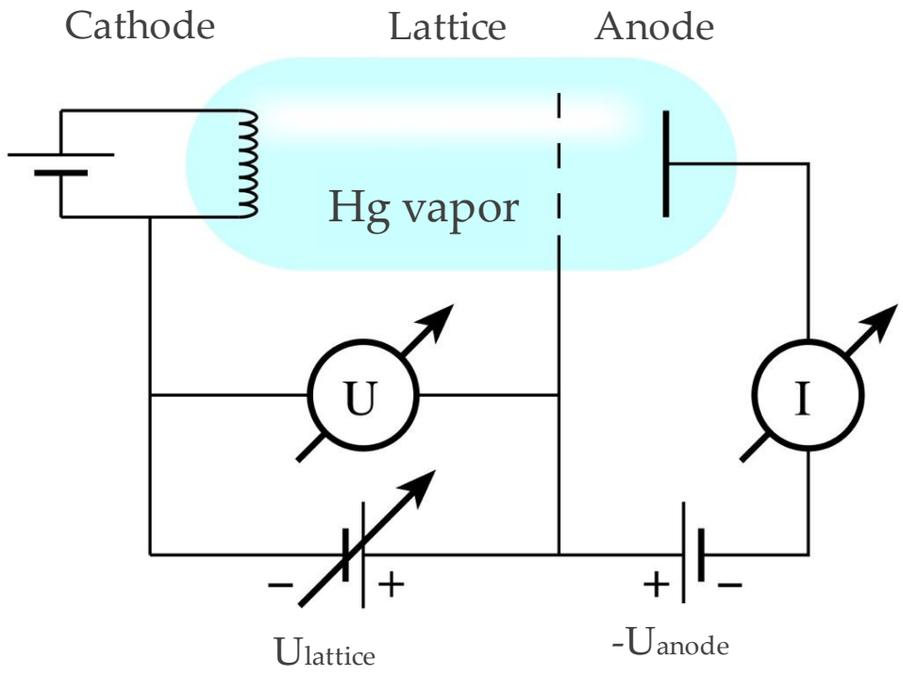
Problem:
-unstable atom
-electrons: centripetal acceleration - light emission - energy loss - falling into the nucleus

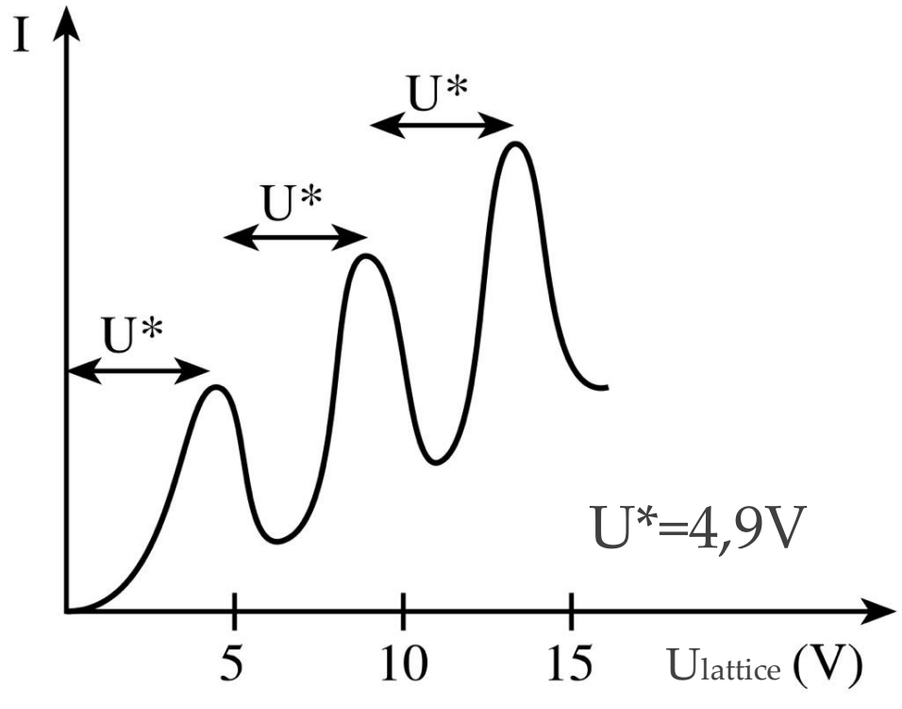
Energy of the atom changes in discrete steps

Franck-Hertz experiment (1914)

James Franck (1882-1964)

Gustav Ludwig Hertz (1887-1875)

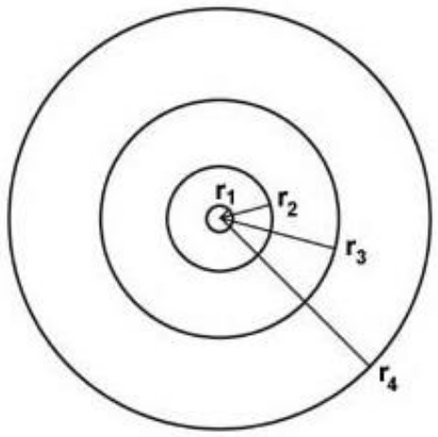




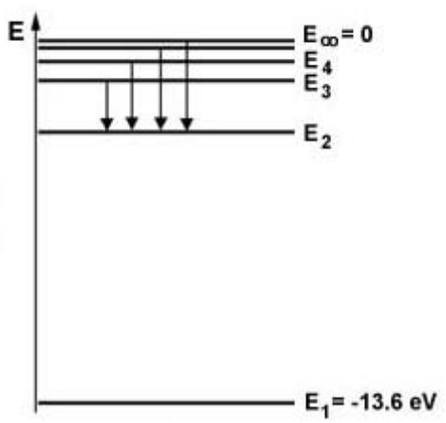
The electrons accelerated by the lattice voltage ($U_{lattice}$), upon inelastic collision with the Hg atoms, loose their energy in discrete packages ("quantum" - sing., "quanta" - pl.).

Bohr model of the atom

Niels Bohr (1885-1962)



Bohr model of the hydrogen atom



Energy levels in the hydrogen atom.

Bohr's postulates

1. Quantum condition:

- The electrons of an atom are on given orbits.
- On the given orbit the elctron does not emit, its energy is constant.
- The angular momentum (L) of the orbital electron is an integer multiple of h/2π:

$$L = mvr = n\frac{h}{2\pi}$$

n= principal quantum number. The radii of the orbits can be calculated.. The radius of the first orbit is $r_1 = 5{,}3\ 10^{-11}$ m ("Bohr-radius"). The radii of the further orbits are:

$$r_n = n^2 r_1$$

2. Frequency condition:

- The atom radiates (i.e., emits light) only if the elctron "jumps" from one orbit to the other.
- Energy of the radiation is the difference between the orbit energies:

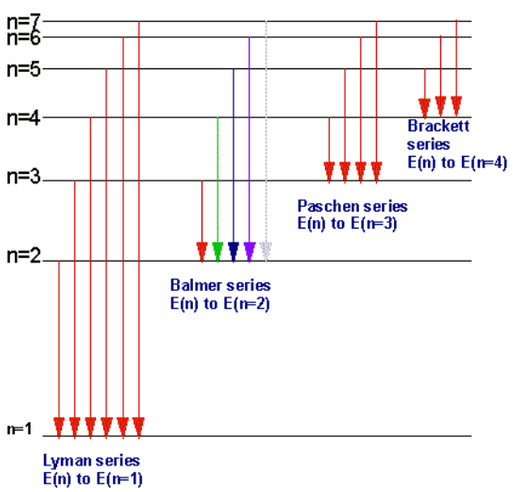
$$E_{foton} = h\nu = E_2 - E_1$$

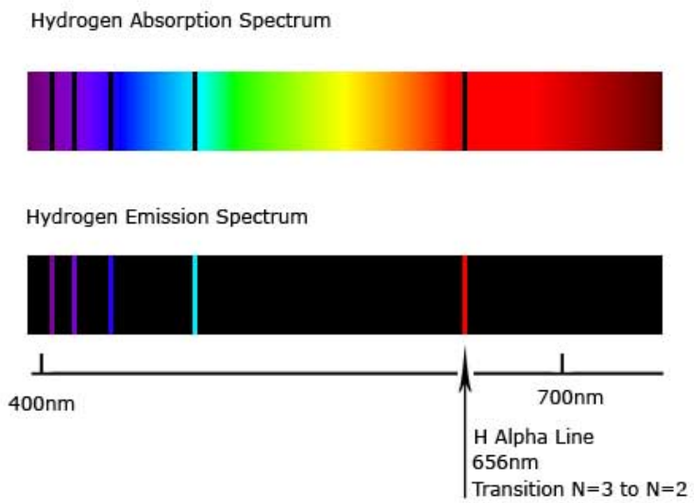
The orbit energies can be calculated. Energy of the first orbit is E_1=-13.6 eV. Further orbit energies are:

$$E_n = \frac{E_1}{n^2}$$

Significance

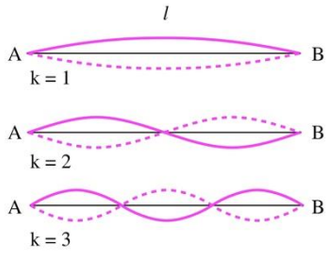
- The model explained the spectra of the hydrogen atom.
  But only that of the hydrogen atom.
- Absorption/emission spectroscopy
- Laser





The electron as a wave

Quantized behavior in the stationary waves of a stretched string

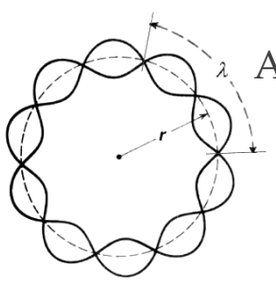


$$l = k\frac{\lambda}{2}$$

The electron as a wave

Louis V. de Broglie (1892-1978)

$$\lambda = \frac{h}{p} = \frac{h}{m_e v}$$



Atomic electron as a standing wave

Quantum condition:

$$2\pi r = n\lambda = n\frac{h}{mv}$$

Propagation law of electron waves

Erwin Schrödinger (1887-1961)

Ψ (psi) wavefunction:

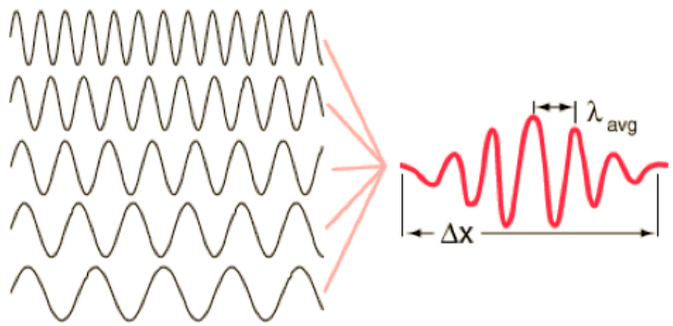
- [Ψ(x,t)]: gives the amplitude of the electron wave as a function of position (x) and time (t).
- Ψ^2: gives the probability of finding the electron.
- Ψ^2: integrated across the entire space = 1 (i.e., the electron can be found somewhere).
- Ψ: with the help of Schrödinger's equation, allows calculation of electron energies.
- For a free electron Ψ is a sine wave: momentum is precisely known (p=h/λ), but position (x) entirely unknown (uncertainty principle!)

Wavefunction of freely moving particle (potential energy = 0)

Uncertainty principle

Werner Heisenberg (1901-1976)

To localize the wave, we need to superimpose waves of different wavelength (λ) (interference):



Upon spreading λ (Δλ), localization will be more certain (Δx decreases), but it also spreads the momentum values (Δp increases), thereby increasing the uncertainty of determining momentum:

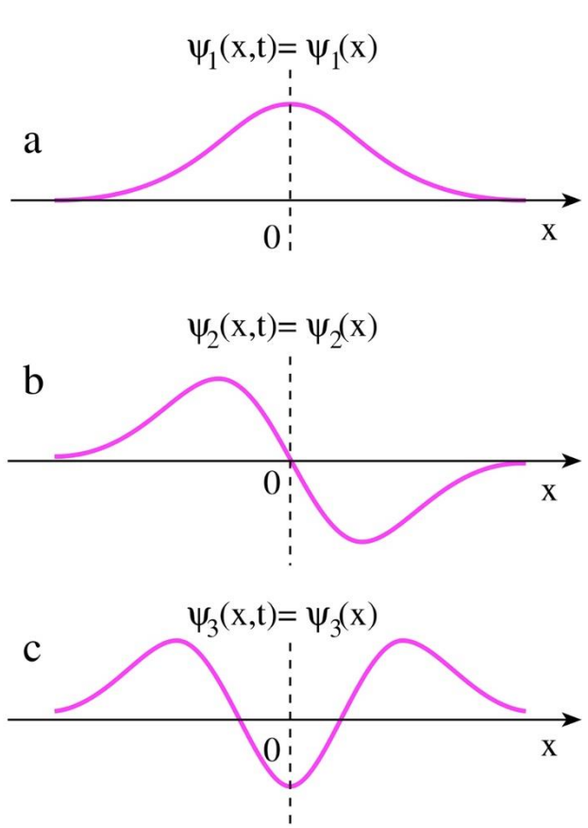
$$\Delta x \cdot \Delta p \geq \frac{h}{2\pi}$$

Quantum mechanical atomic model

Within the atom every electron has a given state, and the probability of finding it around the nucleus has a specific shape.

Quantum mechanics:

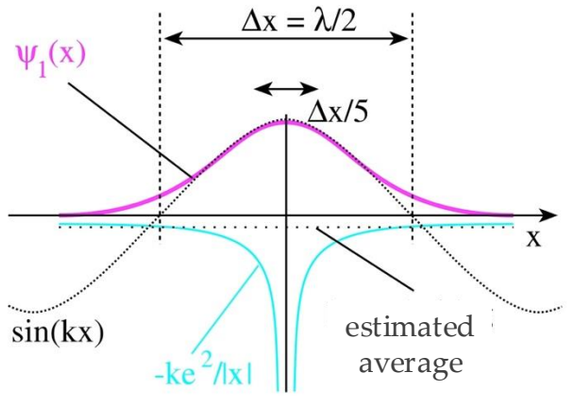
1. describes the states of the electron (one state → one wavefunction, Ψ)



2. calculates the electron's most probable location (orbital, r) and energy (E)

$$E = E_{kin} + E_{pot} = \frac{mv^2}{2} - \frac{e^2}{r}$$

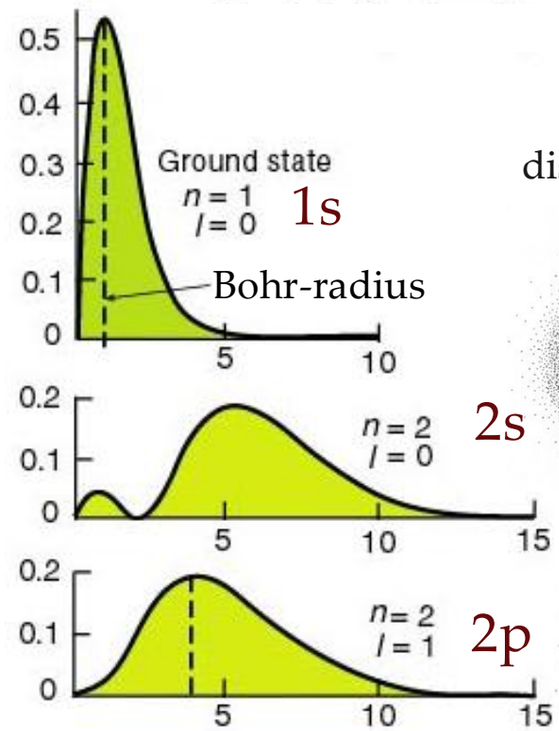
In the atom, Coulombic attraction determines the potential energy:



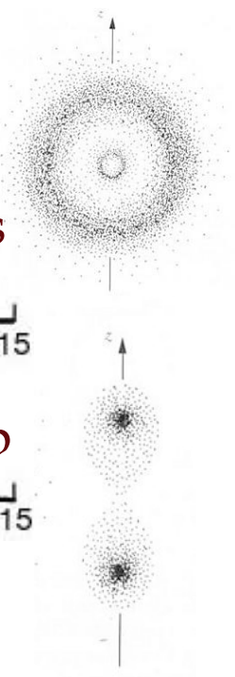
Simplified Schrödinger's equation:

$$\left(\frac{mv^2}{2} - \frac{e^2}{r}\right)\Psi = E\Psi$$

Probability of finding the electron in the atom:



"Spatial distribution"

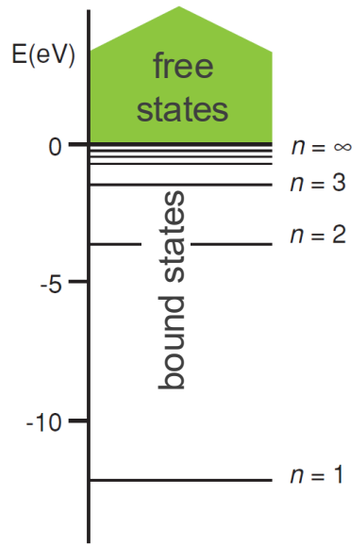


Quantum numbers

The quantum numbers refer to physical quantities that describe the state of the electron:

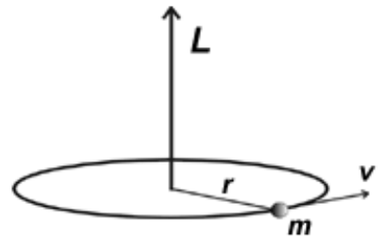
1. Energy

Energy of the electron in a given quantum state

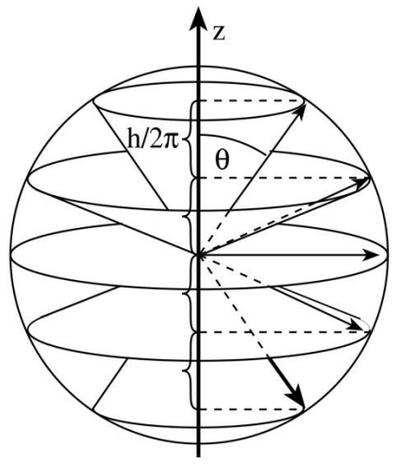


2. Angular momentum

absolute value



direction



3. Spin

Intrinsic angular momentum and magnetic momentum

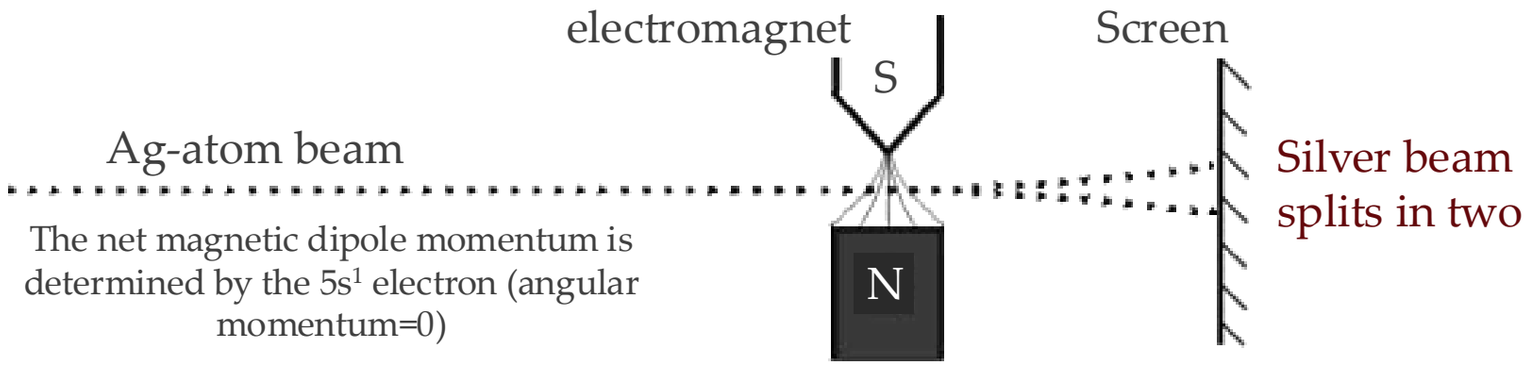
name	symbol	orbital meaning	range of values	value example
principal quantum number	n	shell	$1 \leq n$	$n = 1, 2, 3...$
azimuthal quantum number (angular momentum)	ℓ	subshell	$(0 \leq \ell \leq n-1)$	for $n = 3$: $\ell = 0, 1, 2\,(s, p, d)$
magnetic quantum number, (projection of angular momentum)	m_ℓ	energy shift	$-\ell \leq m_\ell \leq \ell$	for $\ell = 2$: $m_\ell = -2, -1, 0, 1, 2$
spin projection quantum number	m_s	spin	$-\frac{1}{2}, \frac{1}{2}$	for an electron, either: $-\frac{1}{2}, \frac{1}{2}$

The spin quantum number

Otto Stern (1888-1969)

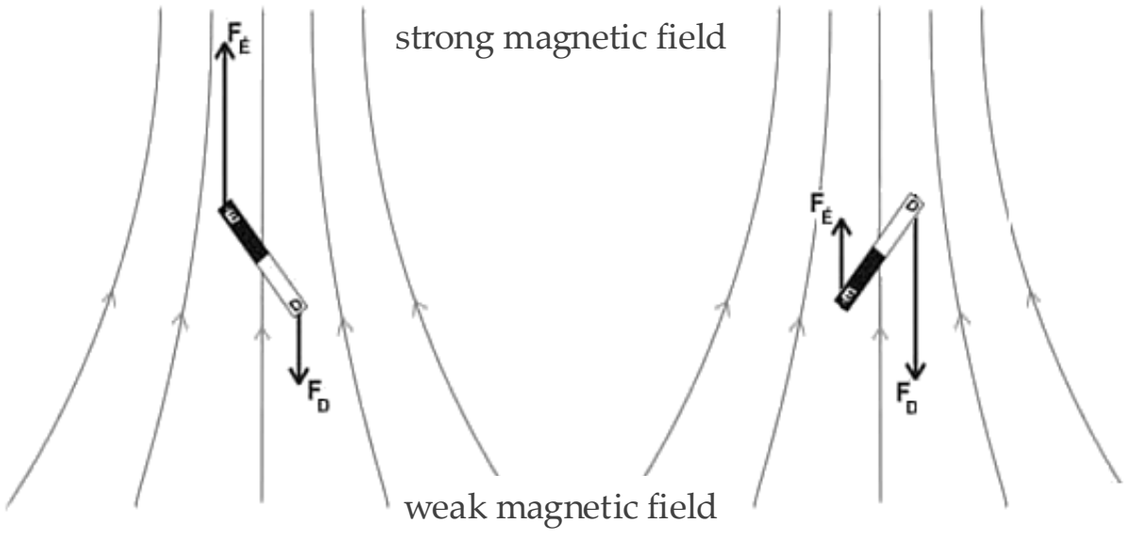
Walther Gerlach (1889-1979)

Stern-Gerlach experiment (1922)

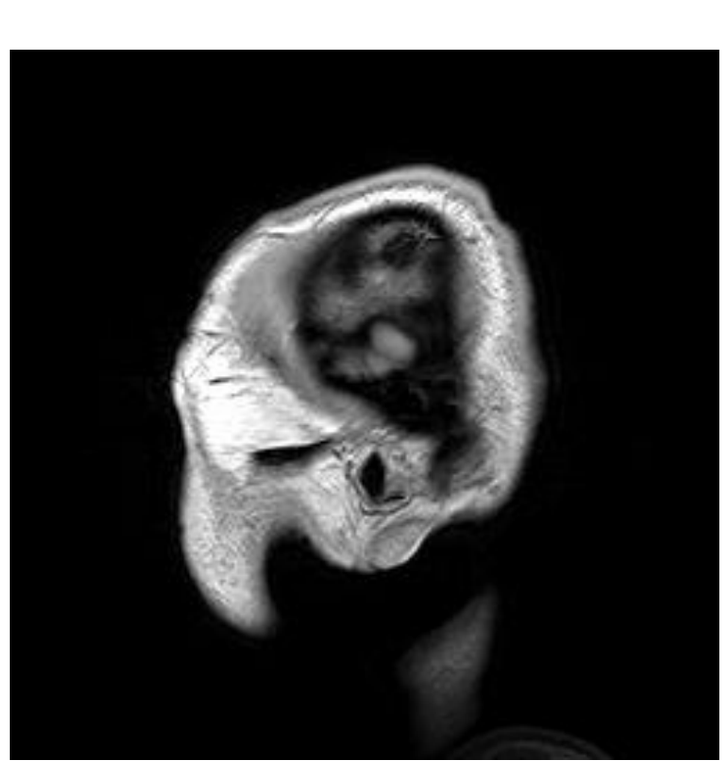


The net magnetic dipole momentum is determined by the $5s^1$ electron (angular momentum=0)

In an inhomogenous magnetic field, in addition to torque, net force arises on the magnetic dipoles:



The spin magnetic moment may take on two values (+1/2, -1/2)



MRI

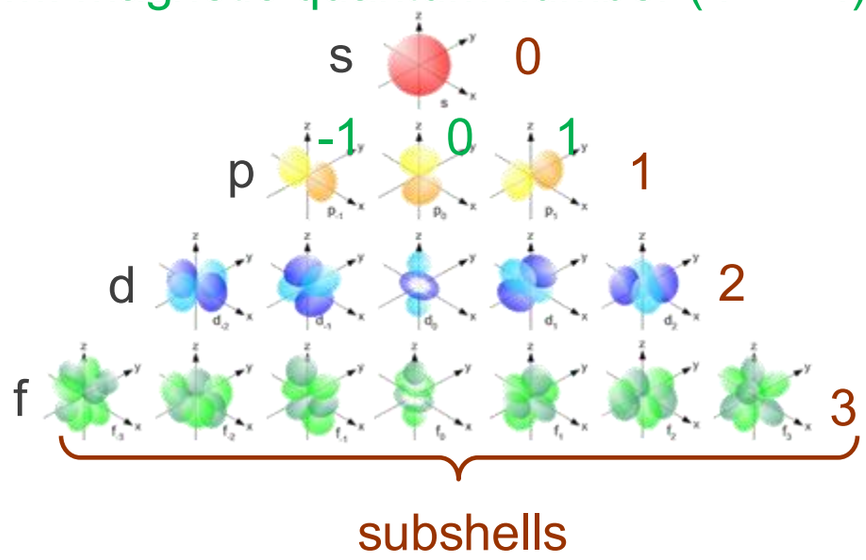
Building up the periodic table

Explicit characterization of the bound electrons: with n, l, m_l, m_s quantum numbers

n → electron shell
n, l → electron sub-shell
n, l, m_l → eletron orbital

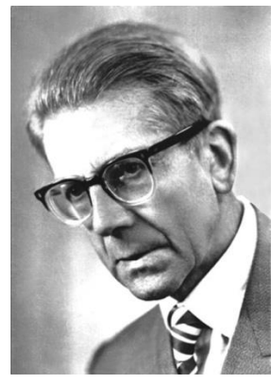
l: azimuthal quantum number (n-1)

m: magnetic quantum number (-*l* → +*l*)



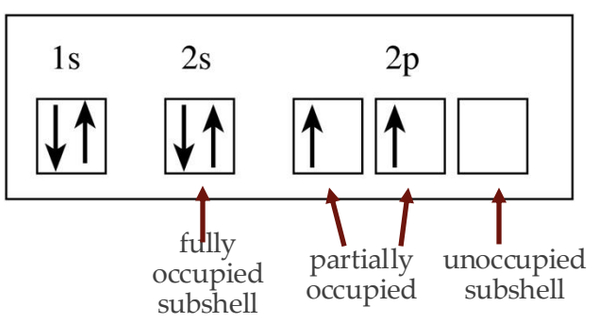
Wolfgang Pauli (1900-1958)

Pauli's exclusion principle:
- Each quantum state can be occupied by a single electron.
- Within an atom there cannot be two electrons for which all four quantum numbers are identical.



Friedrich Hermann Hund (1896-1997)

Hund principle:
- Order of filling up the quantum states.
- For a given electron configuration, the state with maximum total spin has the lowest energy.



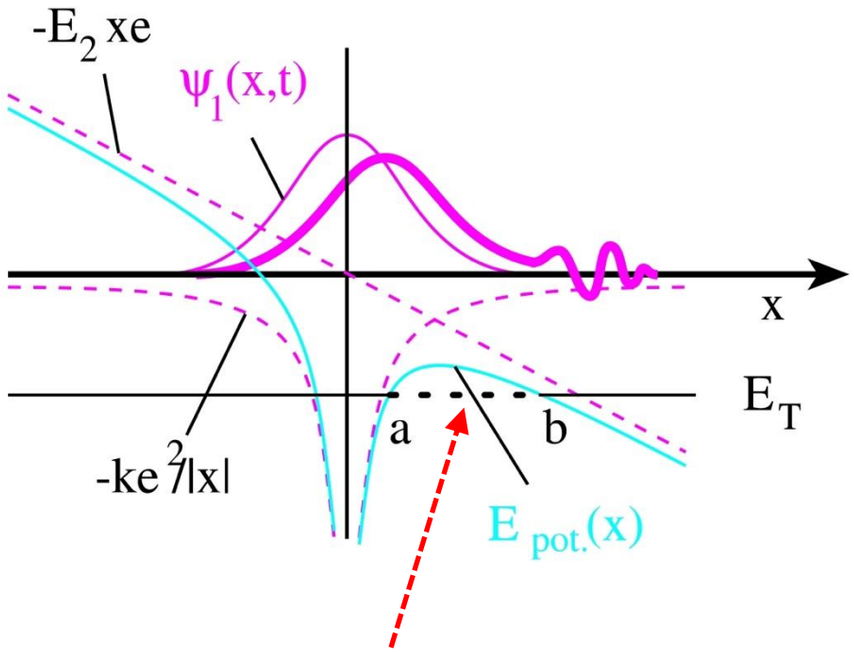
Electron configuration of the C atom
s: "sharp", p: "principal", d: "deformed/diffuse" (spectroscopic nomenclature)

Effect of strong external electric field on the bound electron

The "tunneling" effect

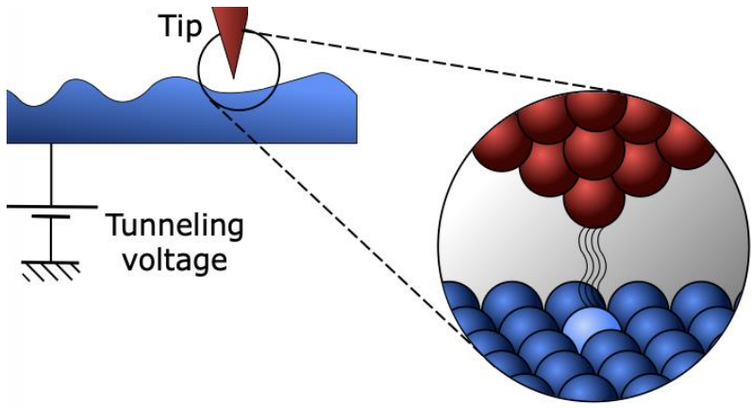
Strong external electric field ($-E_2 xe$):

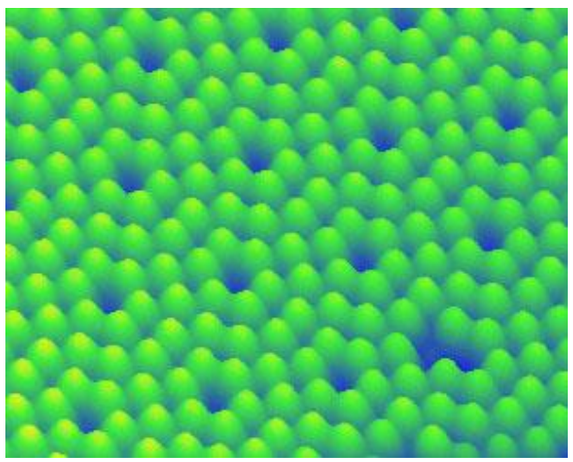
- Ψ is deformed
- The electron may escape the atom without excitation



tunnel through the potential boundary

Scanning Tunneling Microscopy, STM





Si atoms

Tunneling works in macroscopic structures (2025 Nobel-prize in physics)

John Clarke, Michel H. Devoret, John M. Martinis

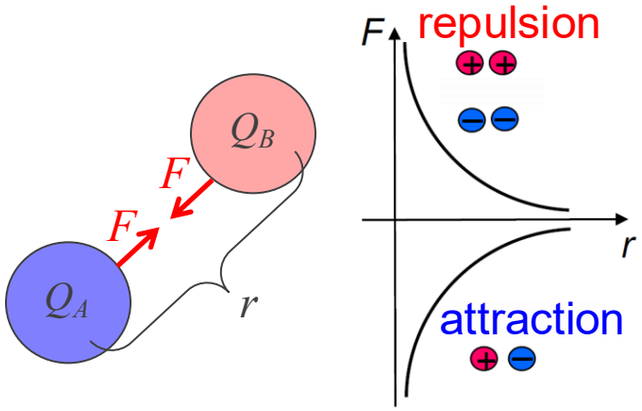
Next generation of quantum technologies:

- quantum cryptography
- quantum computers
- quantum sensors

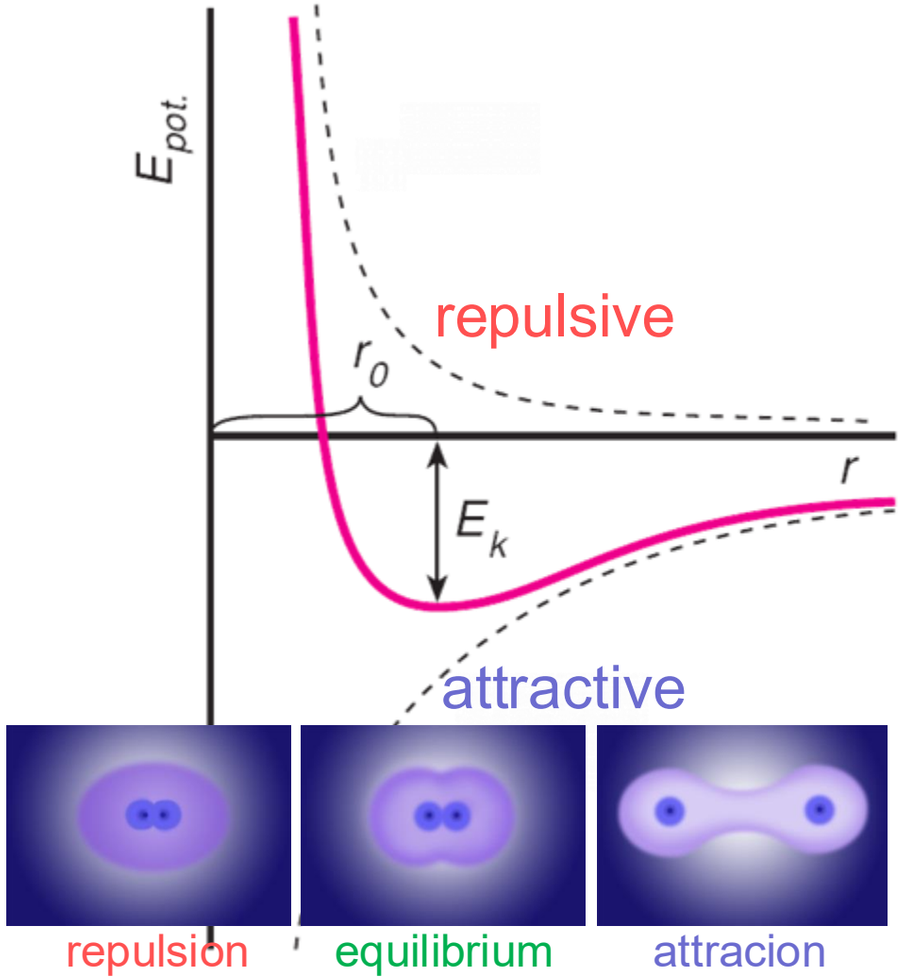
Interactions

Interaction type	Binding particle	Range (m)	Relative strength
gravitation	every particle	infinite (~$1/r^2$)	10^{-40}
electrostatic (Coulomb)	charged particles	infinite (~$1/r^2$)	10^{-2}
strong nuclear	nucleons	10^{-15}	1
weak nuclear	every particle	10^{-18}	10^{-13}

Coulomb-interaction



$$F_C = k \cdot \frac{Q_A \cdot Q_B}{r^2}$$



$$E_{pot} = E_{attraction} + E_{repulsion}$$

$$E_{pot} = -\frac{A}{r^n} + \frac{B}{r^m}$$

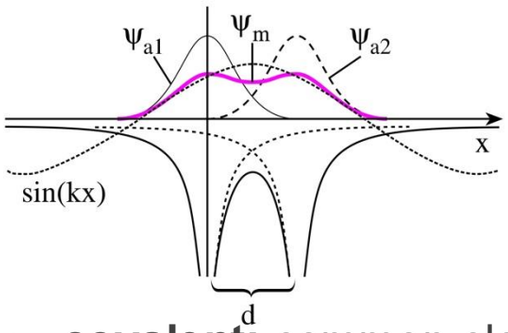
A, B: constants that depend on the interaction and the atoms

n (attraction) < m (repulsion)

r_0: binding distance

E_k: binding energy

Primary bonds



Upon the approach of another proton (nucleus):
- Intermediate Ψ is formed
- The electron belongs to both atoms
- formation of covalent bond

intramolecular ⟷ **intermoleular**

strong ⟷ **weak**

primary ⟷ **secondary**

- **covalent:** common electron state around the participating nuclei, strong: E_b > 1eV
- **metallic bond:** multi-atomic system, E_b > 1eV
- **ionic bond:** Coulomb-forces between ions, E_b > 1eV

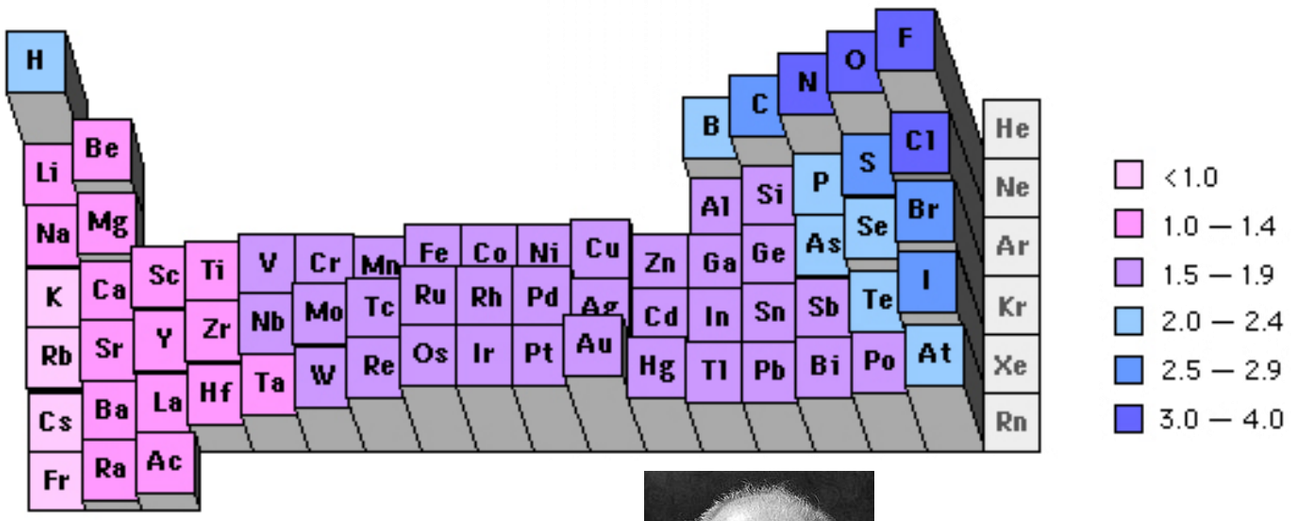
type depends on electronegativity (EN)

EN: tendency of an atom to attract electrons

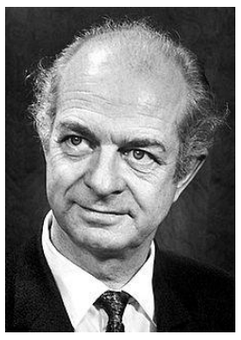
$$EN = |E_i| + |E_{ea}|$$

ionization energy

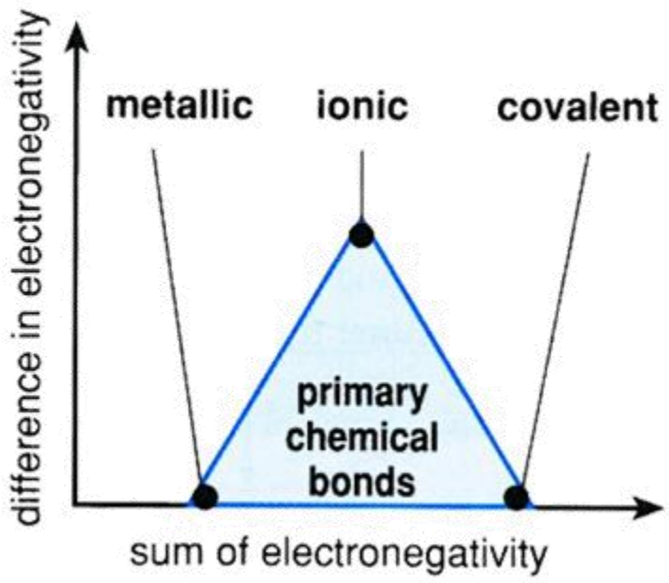
electron affinity



EN values according to Linus Pauling

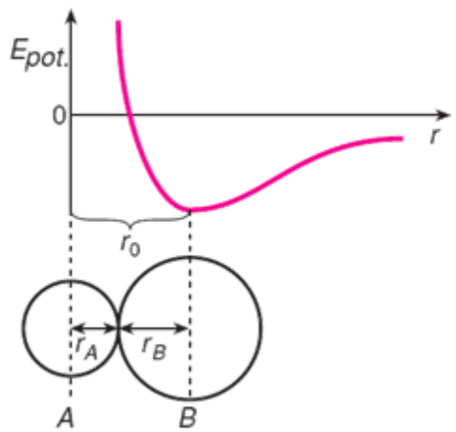


Linus Pauling (1901-1994)

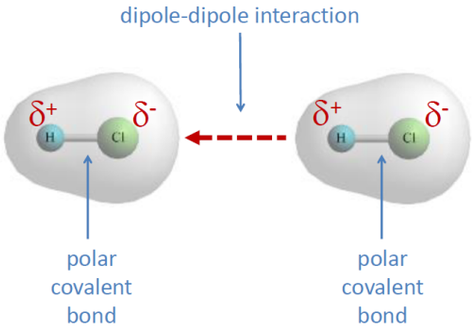


Secondary bonds

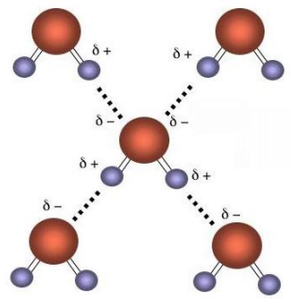
- **Van der Waals:** between two apolar atoms (without permanent dipole moment) where a temporarily created dipole interacts with an apolar molecule or atom thus converting it into a dipole (induced dipole)
  - Van der Waals radius: $r_0=r_A+r_B$
  - Intermolecular or intramolecular
  - Important biological role: formation of organic structures
  - Weak: (E_b ~ 0,02 eV)



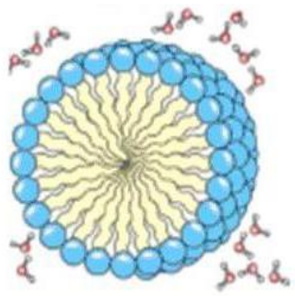
- **Dipole-dipole interaction:** constant charge distribution is present in a (given part of a) molecule
  - partially (+) and (-) segments are held together by electrostatic interactions (Coulomb-forces)
  - intra-/intermolecular
  - weak interaction (Eb = 0.003-0.02 eV)



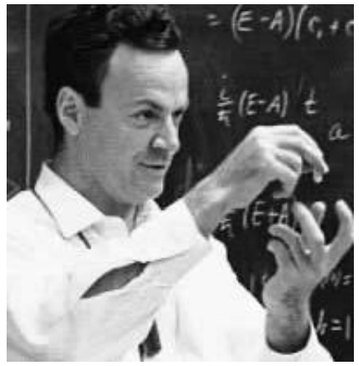
- **H-bond:** H-atom interbridges two other atoms (F, O, N) of high electronegativity
  - r ~ 0,23 - 0,35 nm
  - E ~ 0,2 eV



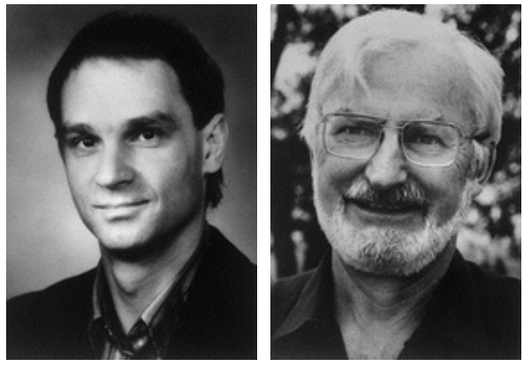
- **Hydrophobic interaction:** weak Van der Waals interaction (Eb = 0.003 - 0.02 eV), thermal motion (kT ~ 0.025 eV) could disrupt the system!
  - ordered water molecules exclude the apolar structures (contact surface can be minimized)



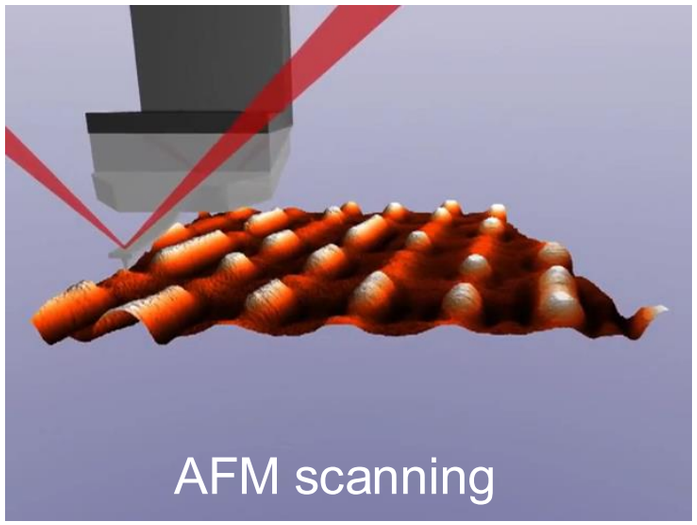
Atomic force microscopy (AFM)



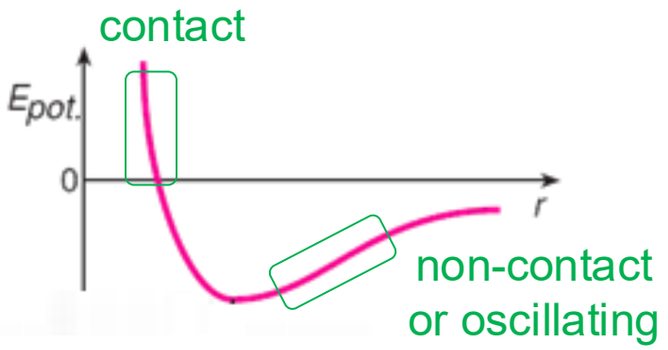
Richard P. Feynman (1959)

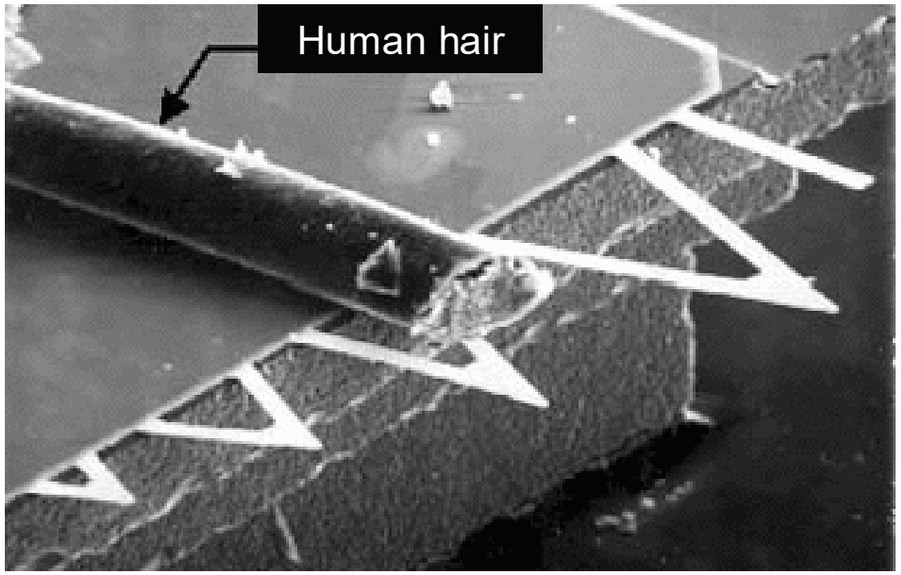


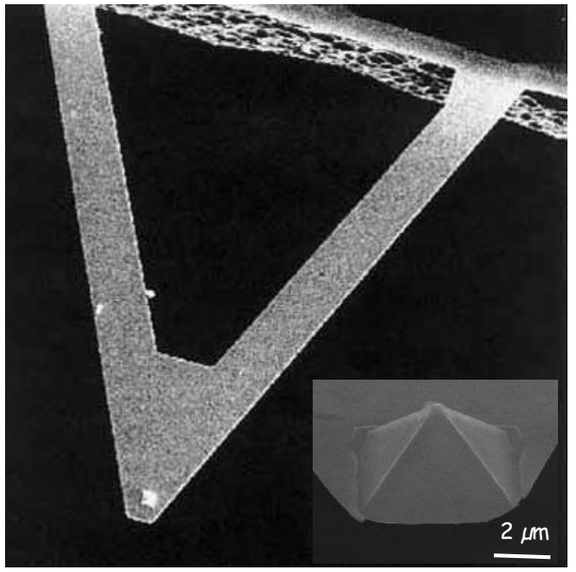
Gerd Binnig Heinrich Rohrer
Nobel-prize 1986

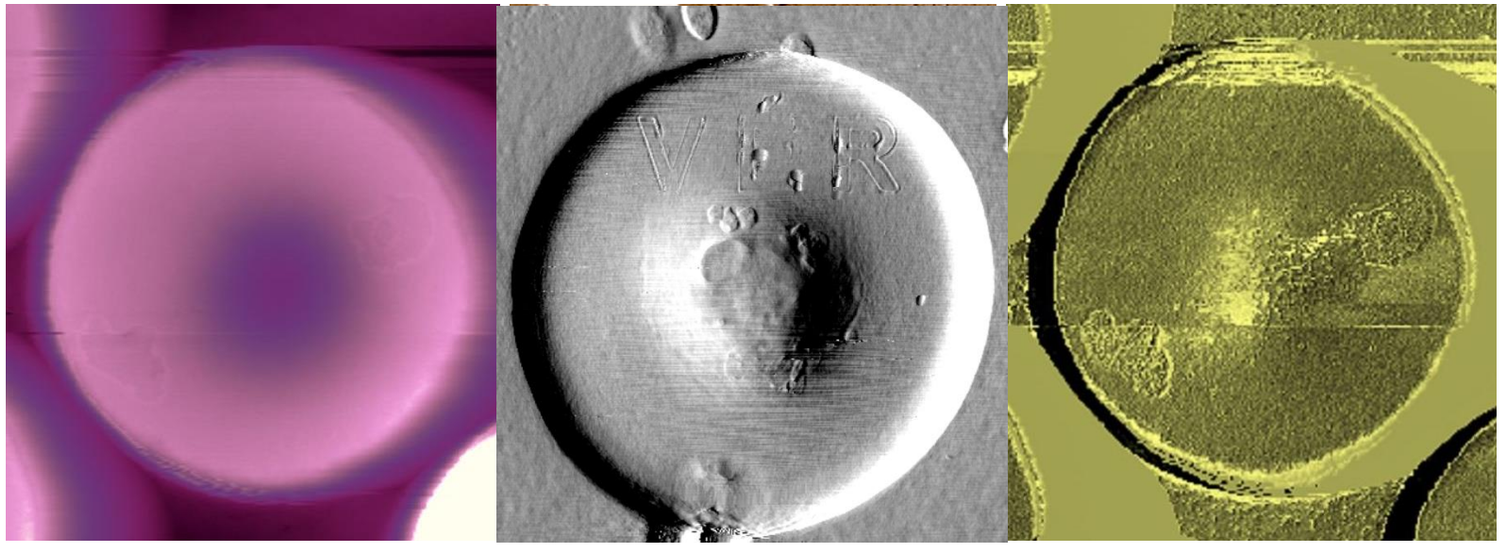


Resolving power of AFM depends on the tip's radius of curvature



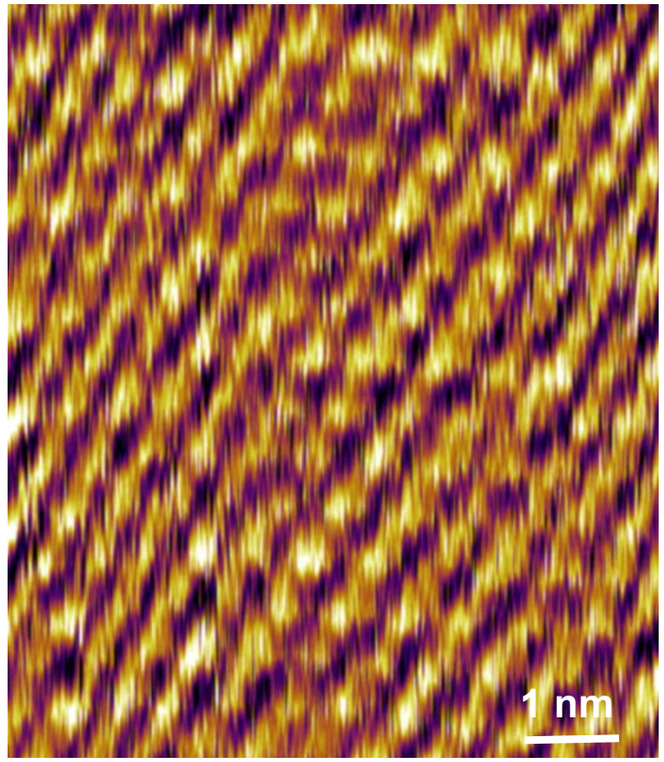




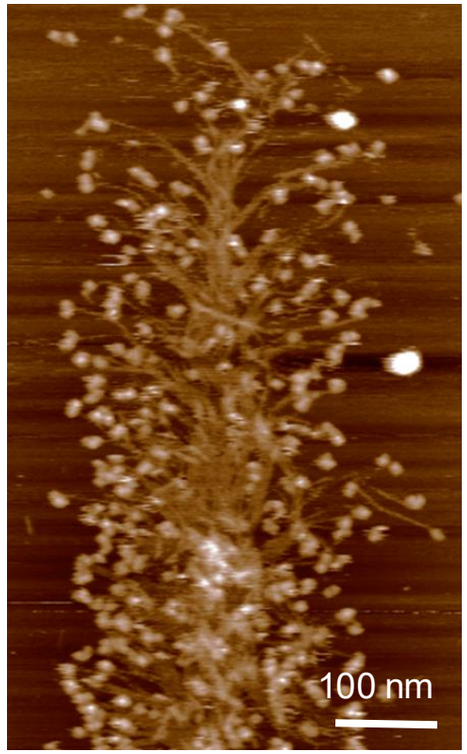


Height contrast Amplitude contrast Phase contrast

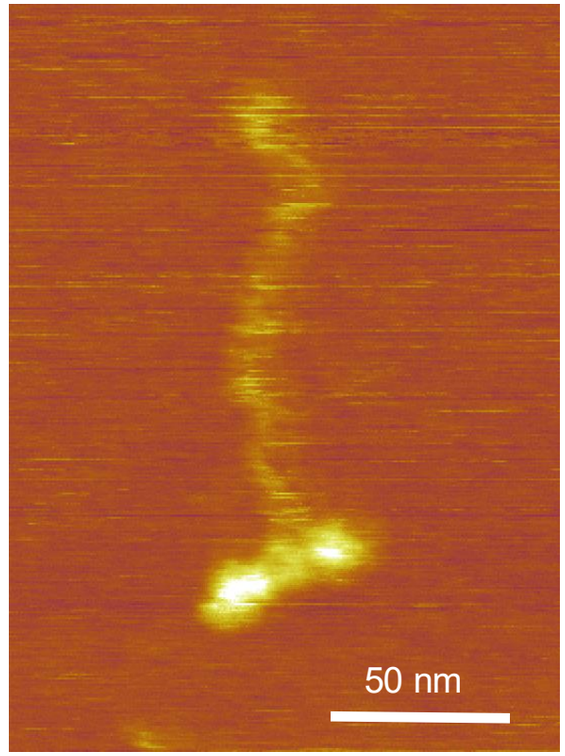
AFM images of nanoscale structures



Atomic structure of mica

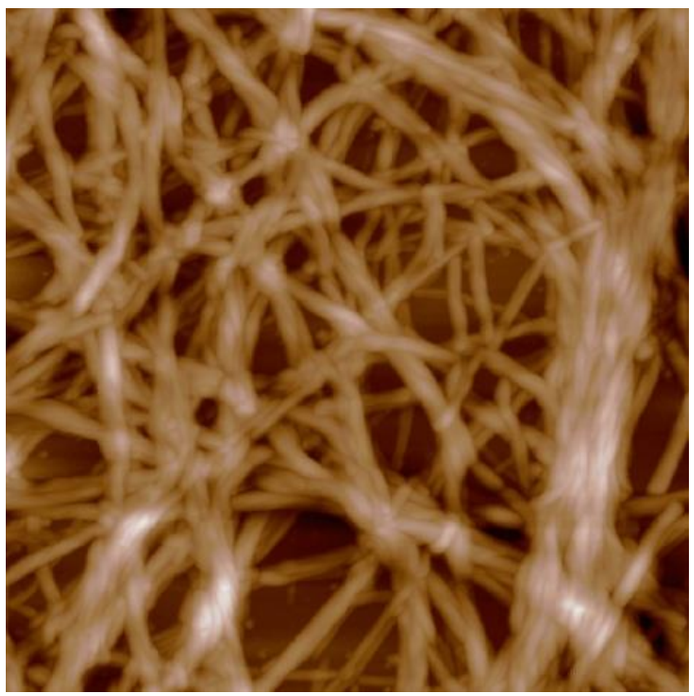


Myosin filament

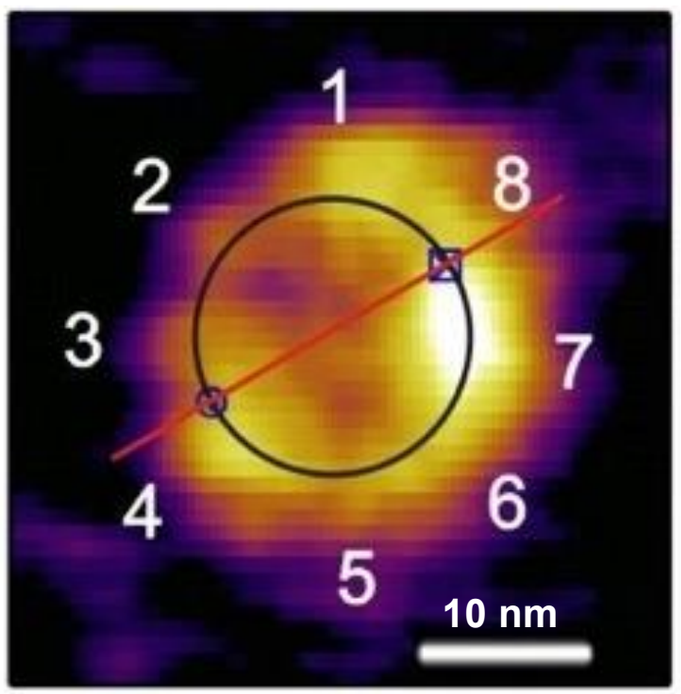


Myosin molecule

Desmin filament

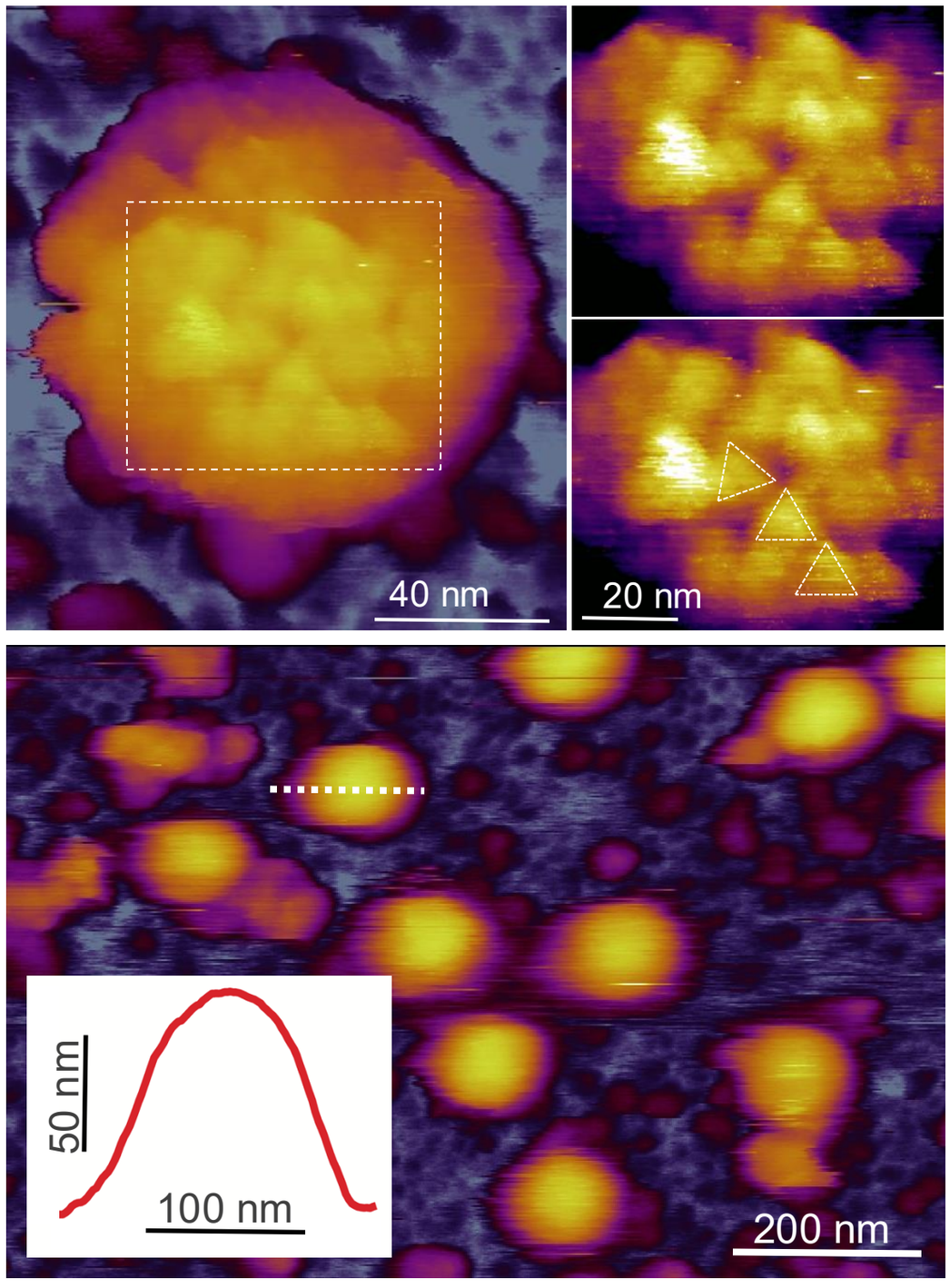


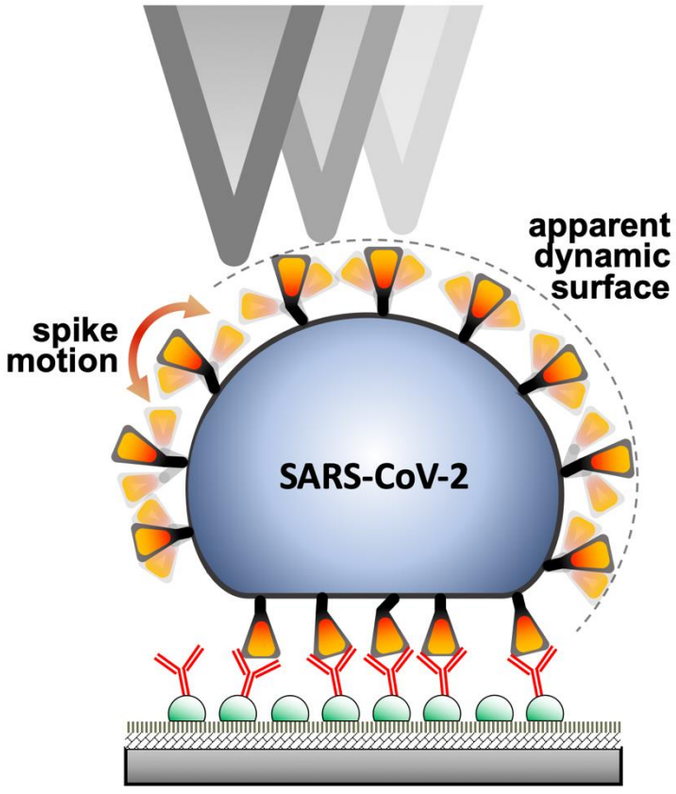
Amyloid ß1-40 fibrils

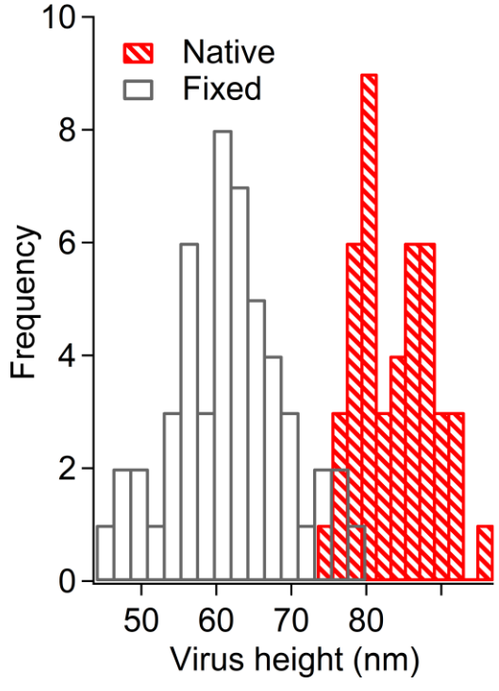


TTR ring oligomer

AFM image (and sound...) of the coronavirus







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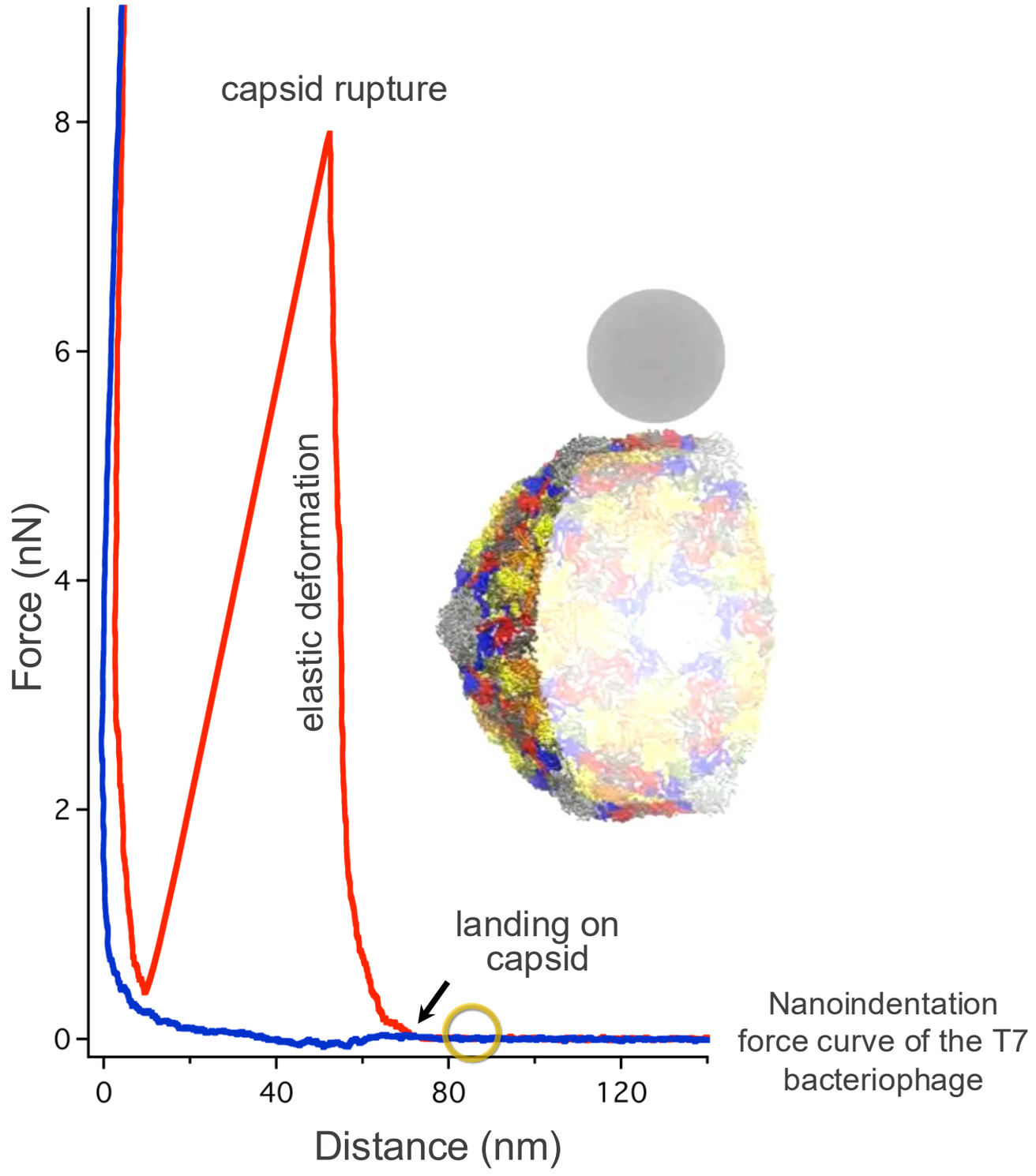
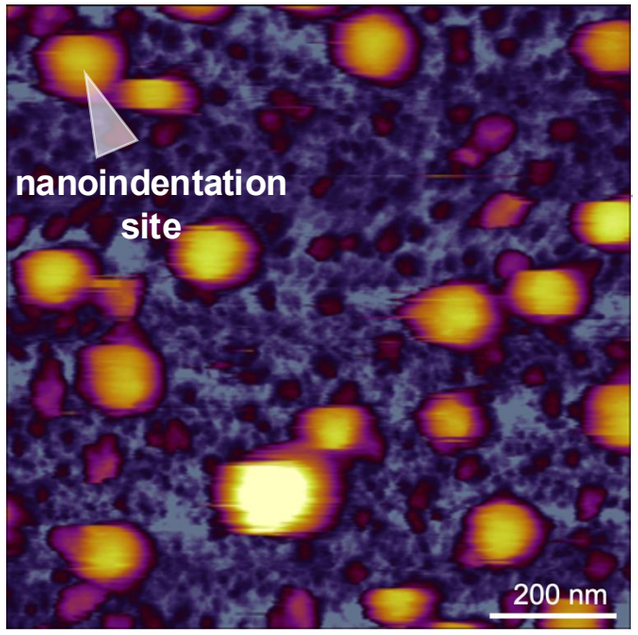
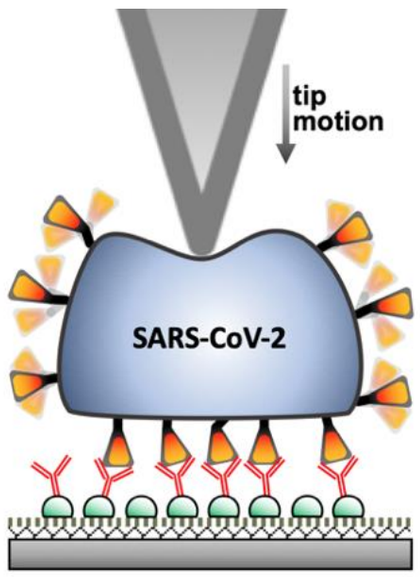
Virus mechanics explored with nanoindentation

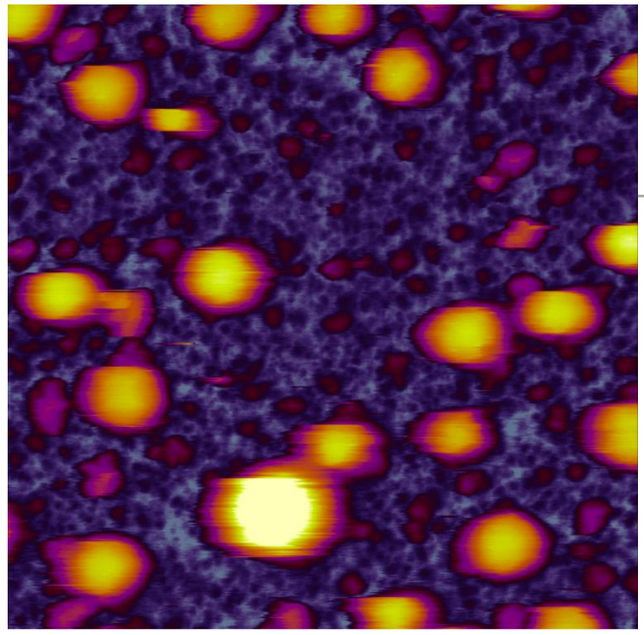


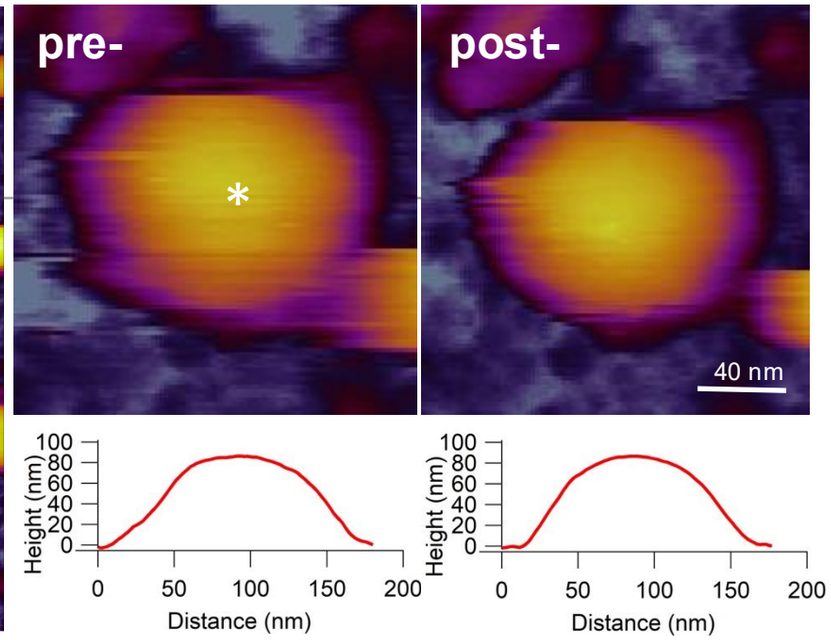
Nanoindentation force curve of the T7 bacteriophage

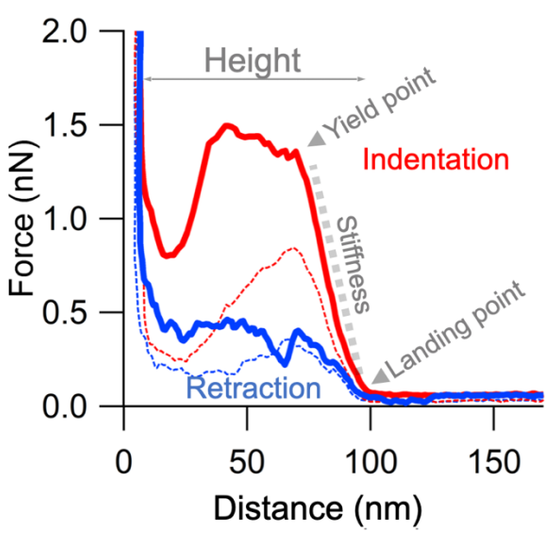
Coronavirus nanomechanics

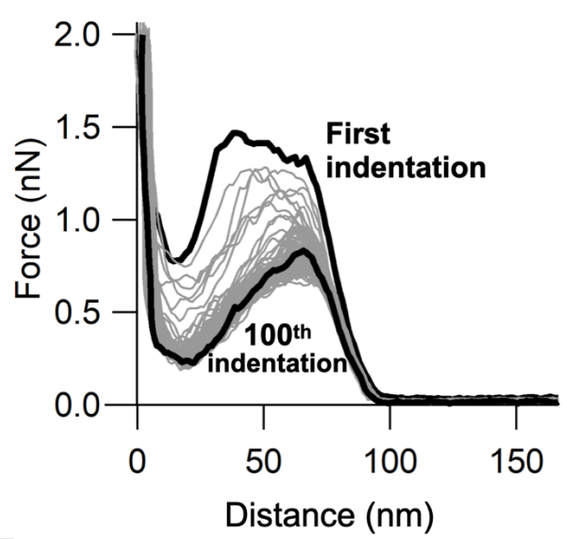


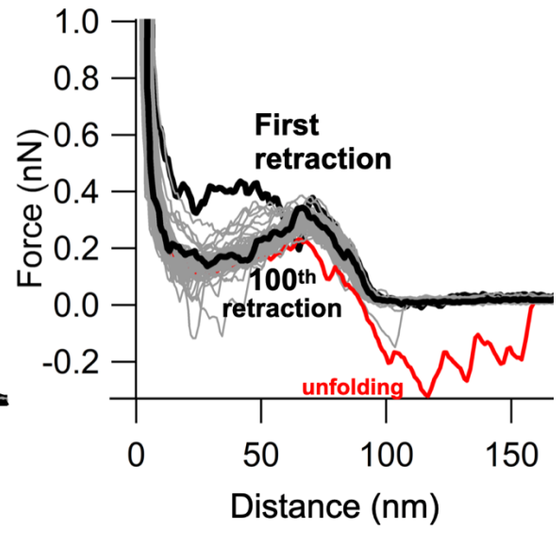




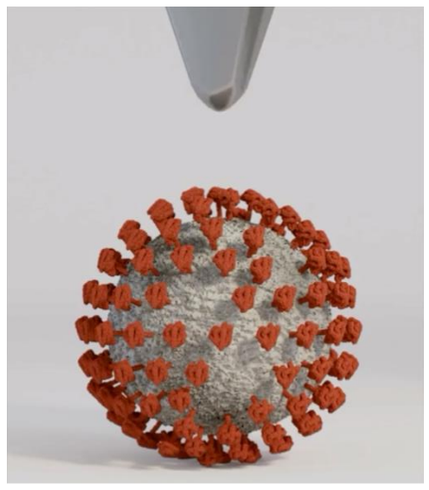


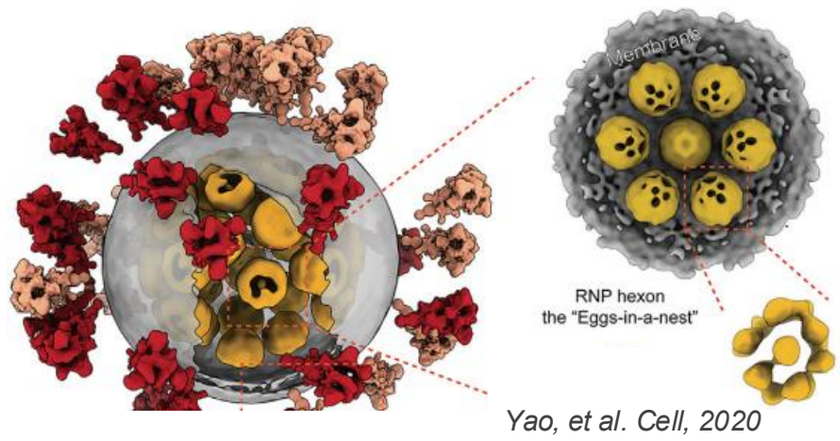






Rubber-ball-like behavior





Yao, et al. Cell, 2020

Kiss et al. Nano Lett 2021

Feedback

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