Advanced Atomic and *Molecular Physics*

Lectures:

Tue: 12:00-14:00
Thu: 10:00-12:00
1.3.14

Ionela Radu

Seminar:

Wed: 14:00-16:00
1.3.14

Christopher Engelhard

The content of the lecture

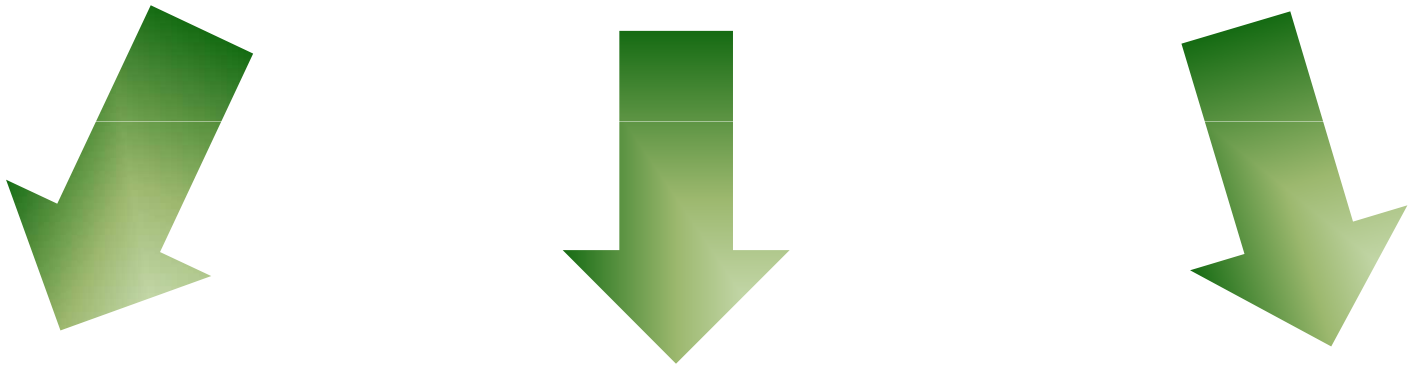
- Repetition: atomic structure
- Molecules: sizes and masses
- Molecular structure: Born-Oppenheimer approximation, valence-bond theory, molecular orbital theory, polyatomic systems, term symbols
- The interaction of molecules with light
- Molecular spectroscopy 1: rotational and vibrational spectroscopy
- Molecular spectroscopy 2: electronic spectroscopy, fluorescence spectroscopy
- Molecular spectroscopy 3: nuclear magnetic resonance, electron paramagnetic resonance
- Single molecule methods: Förster energy transfer (FRET), atomic force microscopy(AFM)

Books:

- H. Haken, H. C. Wolf – Molecular Physics and Quantum Chemistry-Springer
- P. Atkins, J.de Paula – Physical Chemistry – Oxford
- W. Demtröder – Molecular Physics – Wiley-VCH
- P. Atkins, R. Friedman – Molecular Quantum Mechanics - Oxford
- G. M. Barrow – Introduction to molecular spectroscopy – Mc GrawHill
- I.V. Hertel, C.P. Schultz – Atome, Moleküle und optische Physik 2 – Springer
- Handbook of vibrational spectroscopy (vol I-V) – Wiley
- J. Keeler –Understanding NMR spectroscopy- Wiley
- I. N. Serdyuk, N.R. Zacchai, J. Zacchai – Methods in Molecular Biophysics - Cambridge

The Goal of Molecular Physics

... is to learn about and to understand the **structure**, the **chemical bonding**, and the **physical properties** of **molecule**s in all their variety.



Functions **Reactions** **Effects**

of molecules in physico-chemical, and biological systems.

What is particular about molecules?

The molecule is the smallest unit of a chemical compound which still exhibits all its properties.

The system: N nuclei $+$ $\sum_{i=1}^{N} Z_i$ electrons

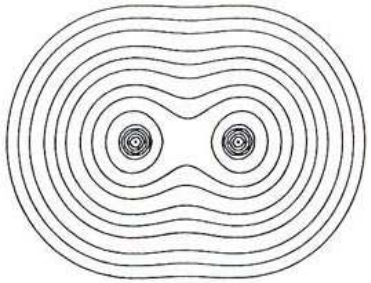
Clasically, a molecule with : N atoms $\Rightarrow 3N$ nuclear degrees of freedom:

$$\begin{cases} 3 & \text{translation} \\ 3 & \text{rotation} \\ 3N-6\,(5) & \text{vibration (linear)} \end{cases}$$

The simplest molecules are **diatomic** and:

• **homonuclear** as **H_2, N_2 or O_2**

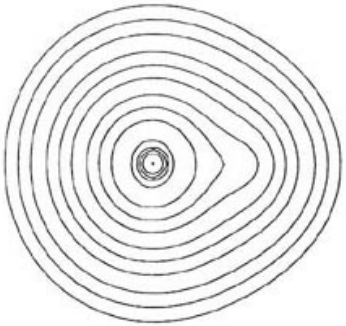
(covalent / homonuclear bonding)



O_2

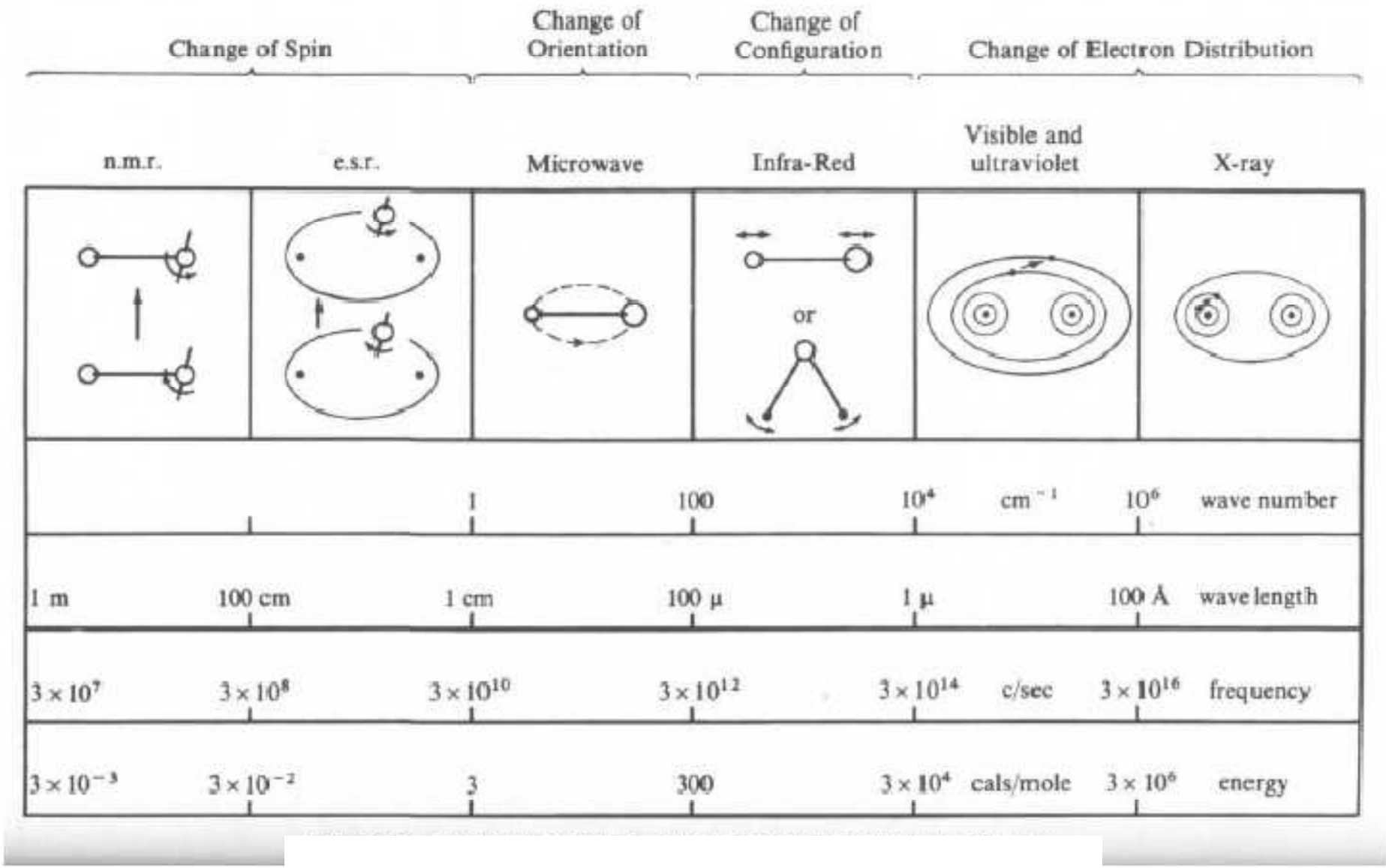
• **heteronuclear** as **LiF, HF or CO**

(polar / heteronuclear bonding)



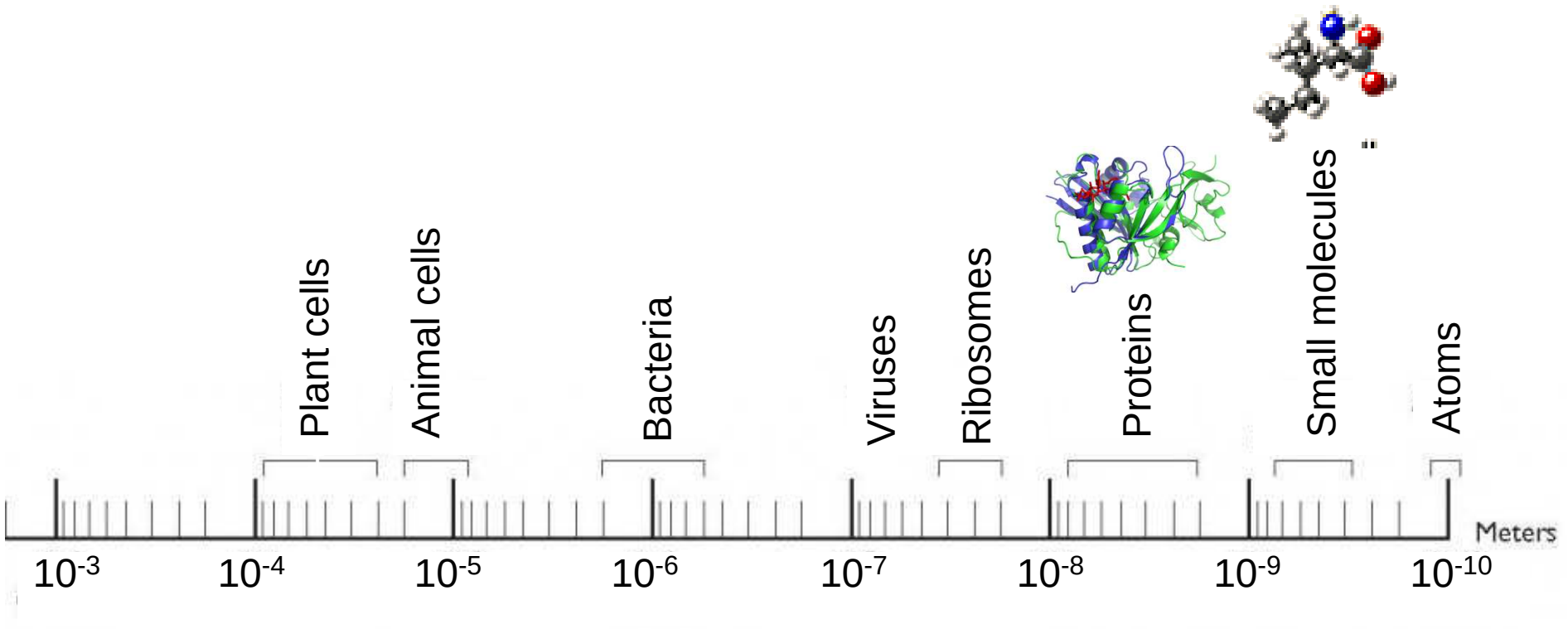
HF

Types of molecular spectroscopy



1 eV = 23.06 kcal / mol

Molecular sizes

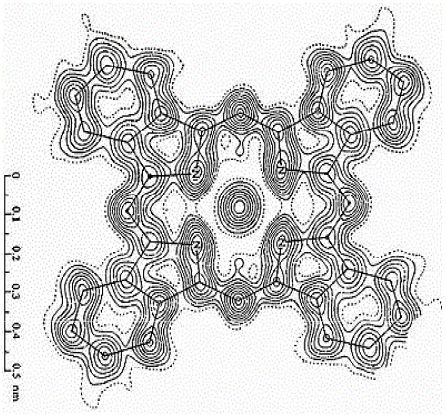


Methods of determining molecular sizes

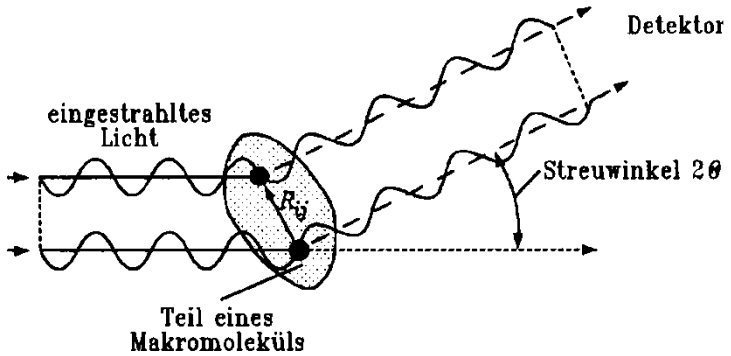
- measurements of transport properties in the gas phase: diffusion, viscosity, or thermal conductivity.

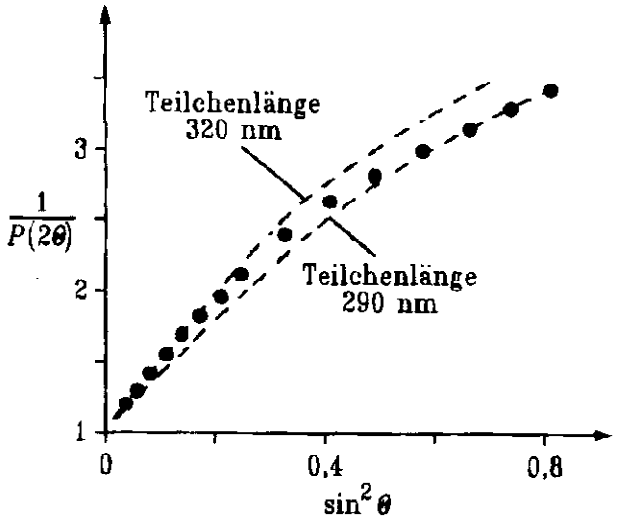
Molekül	d(Å)
H_2	2,3
O_2	3,0
CO_2	3,4
C_2H_6	3,8

- X-ray or electron difraction on single crystal samples



- light scattering

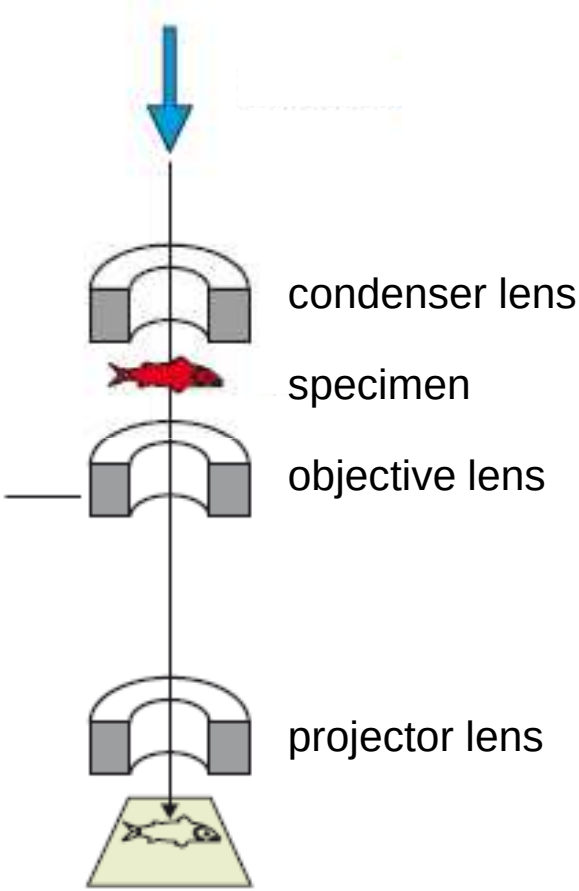




Light scattering of tobacco mosaic virus: length of ~ 300 nm.

Microscopic images of molecules

- transmission electron microscopy



acceleration voltage :

1 kV

10 kV

100 kV

de-Broglie wavelength:

$\lambda = h/mv$

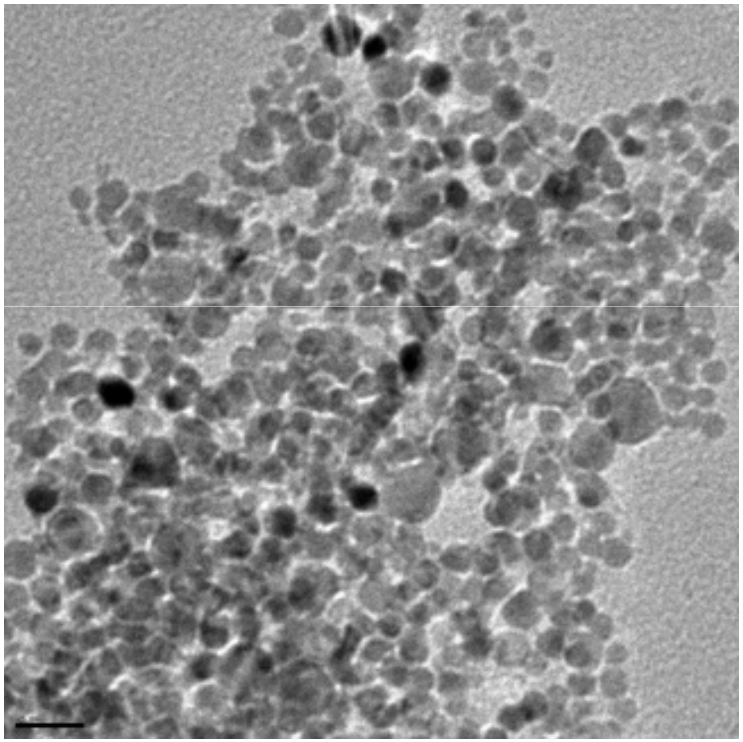
0.04 nm

0.012 nm

0,0037 nm

Spatial resolution:

$d_{min} = C_S \times \lambda^{3/4}$

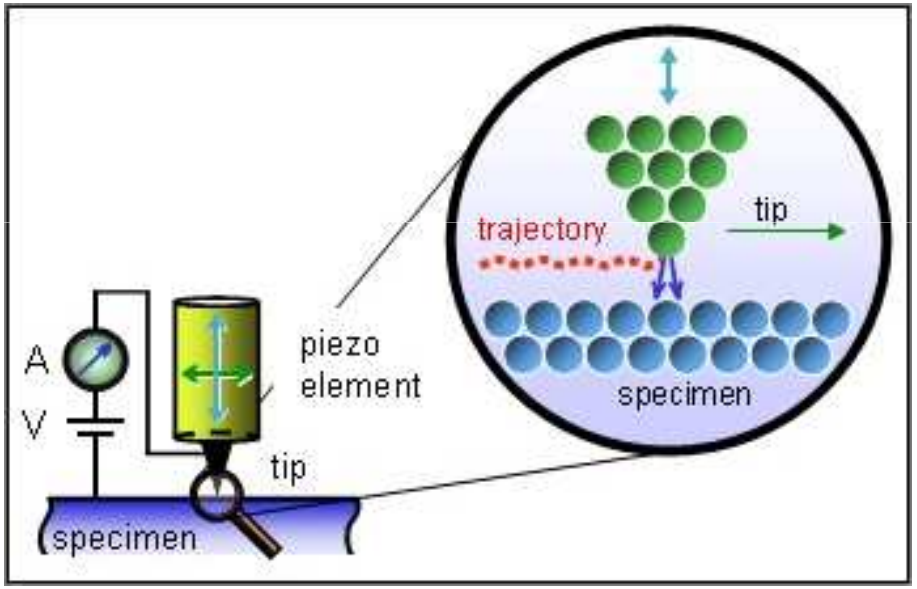


TEM of silver nanoparticles; scale bar is 20 nm

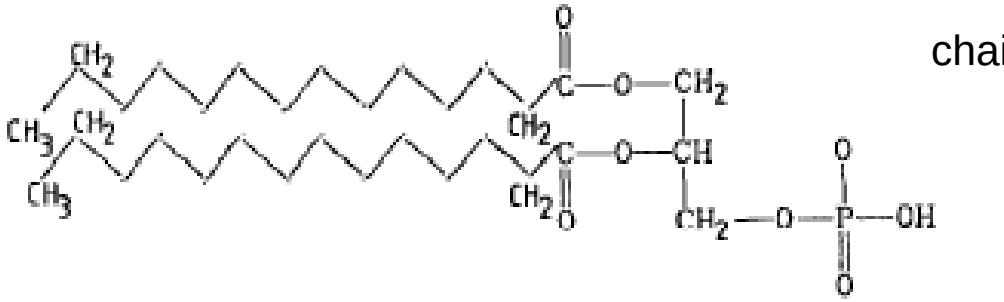
Microscopic images of molecules

- scanning tunneling microscopy:

invented by **Gert Binnig and Heinrich Rohrer (**IBM Zürich)
1986 Nobel prize

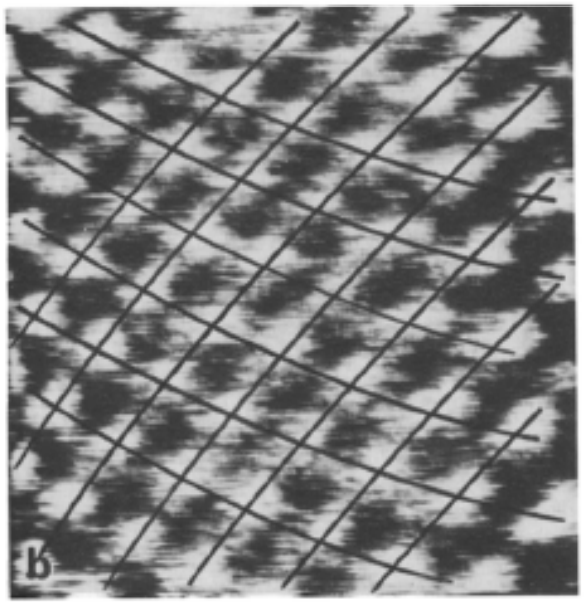


scanning tunneling microscopy:
STM image of DMPA layers adsorbed on a graphite surface

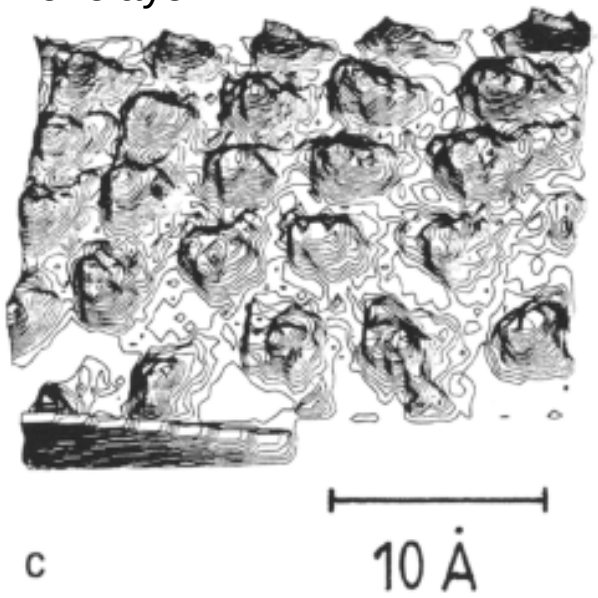


chain-chain distance: 4.3-5.3 Å (STM)
4.15-4.3 Å (X-ray diffr.)

bilayer



monolayer

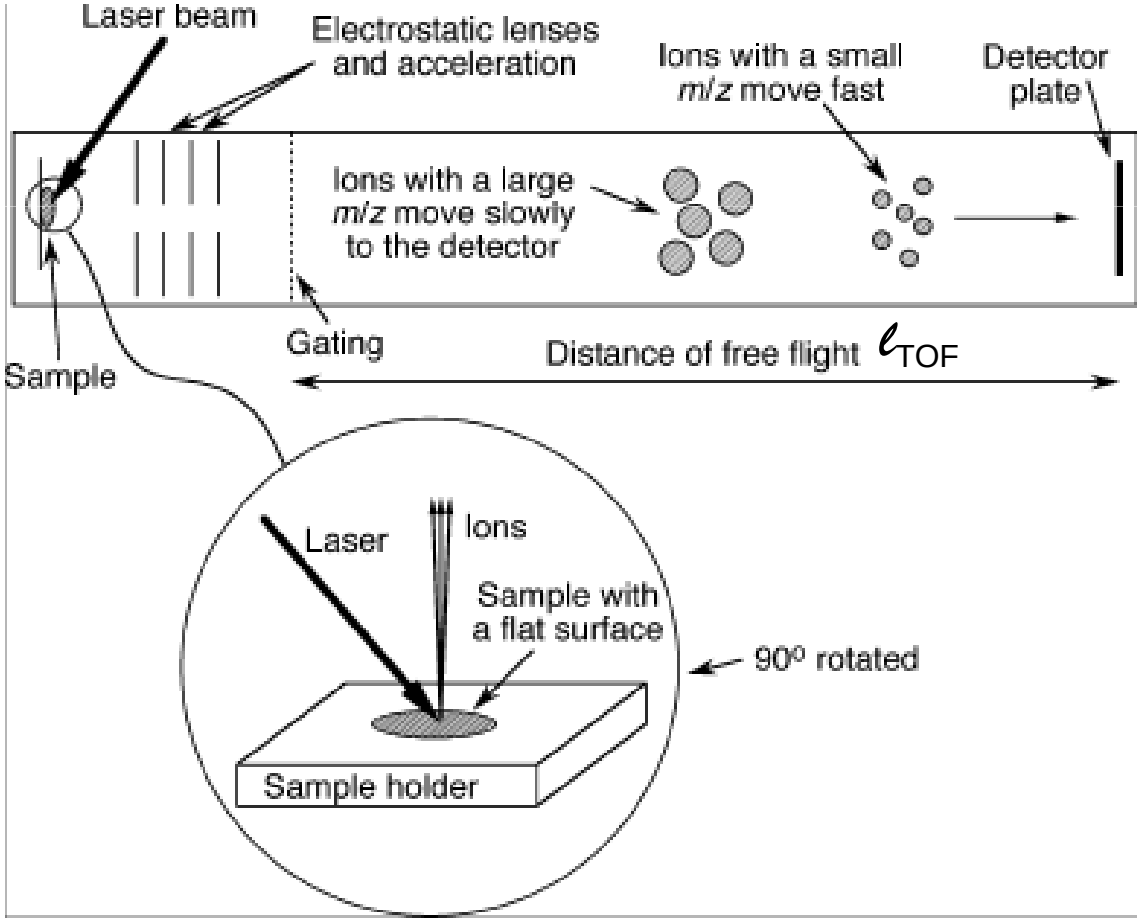


Hörber et al., *Chem Phys Lett* 145, 1988

Molecular masses

Molecular mass: measured in daltons (Da) or atomic mass units (amu)
1 Da = 1 amu = 1/12 m(^{12}C) = 1.660538921(73)×10^{-27} Kg

• **Mass spectrometry: MALDI-TOF**
(matrix assisted laser desorption/ionization coupled with time of flight detector)



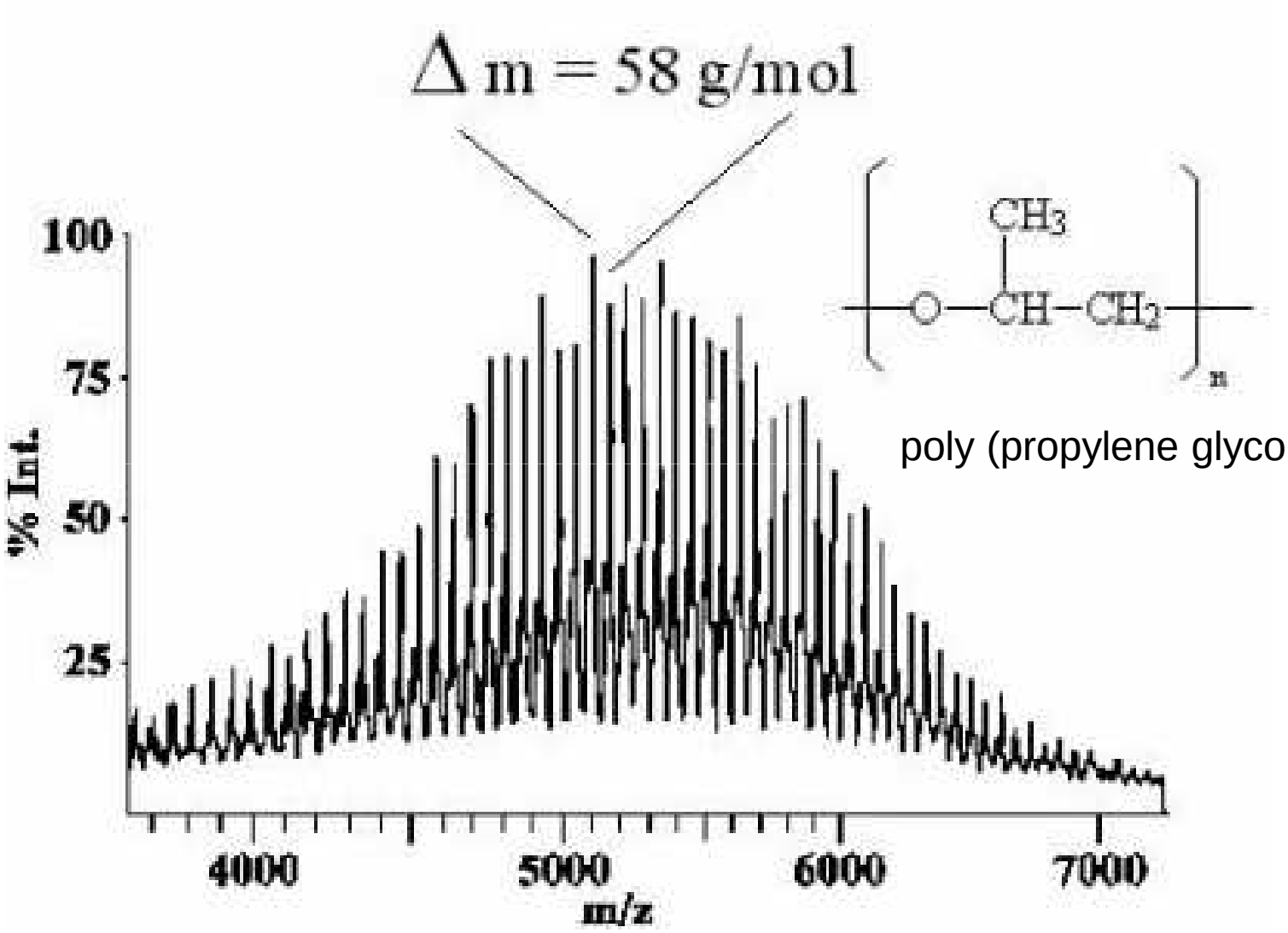
Kinetic energy of an ion:
(m mass, z charge, V voltage)

$$E = zV = \frac{mv^2}{2}$$

Time of flight:

$$t = l_{TOF}\sqrt{\frac{m}{2zV}}$$

Molecular masses: MALDI-TOF Spectra



poly (propylene glycol)