Finite Ring Geometries and Role of Coupling in Molecular Dynamics and Chemistry

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FINITE PROJECTIVE RING GEOMETRIES

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Outline of the talk

Changes (evolution in time) – quantitative / **qualitative**

Quantitative approach ~ approximations
Examples – elementary systems of classical / quantum mechanics, complex systems (many body $\rightarrow$ ‘living’ systems)

Qualitative changes – implications for space and time
$\Rightarrow$ hierarchic build-up principles

Possible contribution from the non-continuous (discrete step) approach

Static vs. dynamic approach

Conventional approach in physics / chemistry –
certain combination of a **static** and **dynamic** approaches

Static ~ existence of elementary building blocks primarily assumed (in **space** - 3D, phase space, …)

Dynamic ~ interaction by forces (electromagnetic, gravitational) derived from properties of matter (charge, mass)

Motion in **time**

Laws of physics – laws of conservation, continuous symmetry
Infinitesimal calculus (point mass, point charge)

Laws of conservation

Laws of conservation – linear equations of motion, closed systems, continuous changes

- Energy ↔ translation in time
- Momentum ↔ translation in space
- Angular momentum ↔ rotation in space

Continuous change – only quantitative nature, two infinitesimally close points in space / time cannot be regarded as qualitatively 'different'

Qualitative change

In such a setup – a conceptual problem with describing any **qualitative** change (~ formation of a system of bound particles)

Difficulties with the notion of **time**
'Evolution' according to physical laws ~ reversible time, describes only quantitative changes, absence of qualitative changes

Qualitative change ~ **arrow** of time

?

Such change of the nature of **time**
⇓
Change of concept of **space**

Qualitative change

? Can a **qualitative** change be described within a **continuous** concept

Qualitative change – emergence of new properties
atoms → molecule : center of mass, moment of inertia, vibrational frequency

? Can a **qualitative** change be described within a concept of a **closed system**

Should be perhaps considered together with the continuous / discrete issue

Qualitative change

Qualitative change described in a closed system

Need of some additional assumptions which are not part of the physical model - examples

Classical mechanics - nonlinear model (with driving force, damping)

Quantum mechanics – introducing the spin of electrons in the bonding orbital of the hydrogen molecule H_2

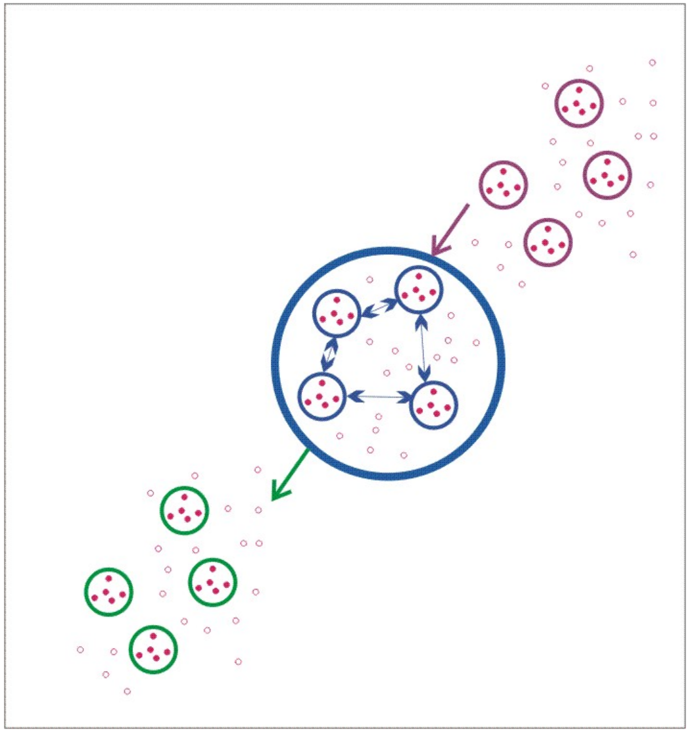
Characteristics of ‘living’ systems

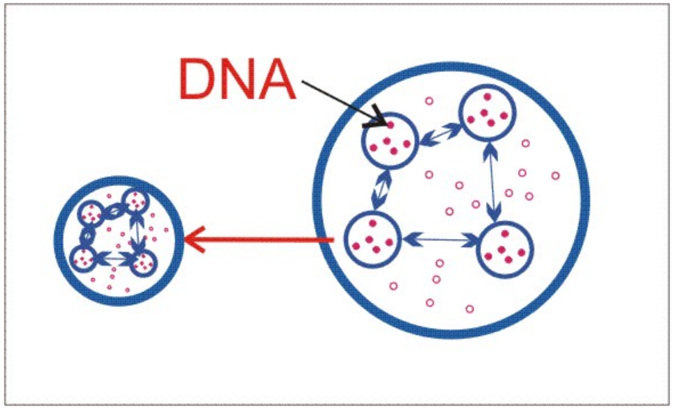
Living systems (LS) exhibit certain properties of behavior which are difficult (impossible) to be described by extrapolations of fundamental physical (chemical) models to situations which do not treat the influence of their surroundings (environment) as a mere perturbation

- Exchange of energy and matter with their surroundings that does not lead to their ‘rapid’ disintegration (spontaneous, in the sense of the 2^{nd} law of thermodynamics)
- Reproduction (production of offsprings)

Characteristics of ‘living’ systems

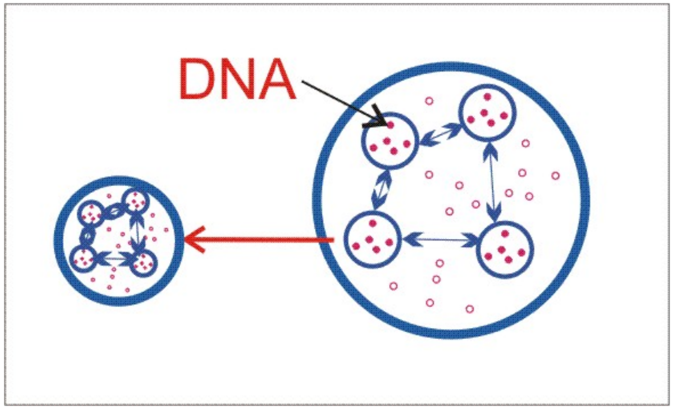
i) Exchange of energy and matter with their surroundings



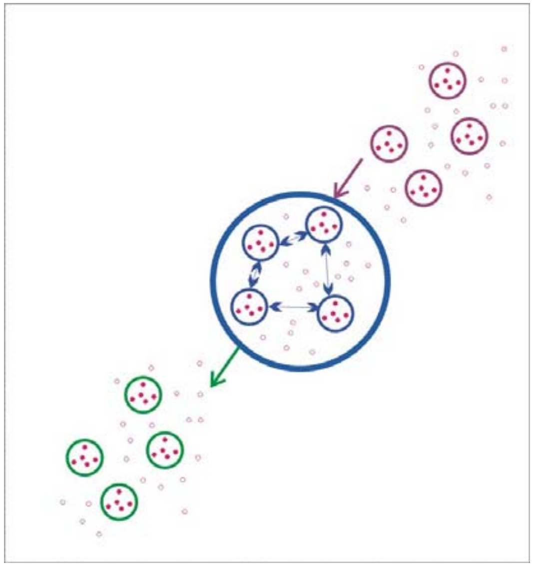


ii) Reproduction (production of offsprings)

Characteristics of 'living' systems

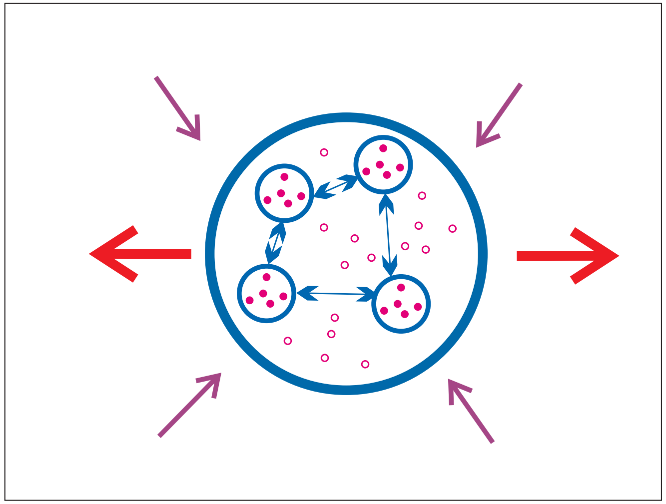


Reproduction - use of information (DNA) ~ gathered in the course of evolution and stored in a **very stable**, **structurally specific**



Metabolism - DNA provides a prescription for synthesis of proteins used in cell chemistry

Characteristics of ‘living’ systems



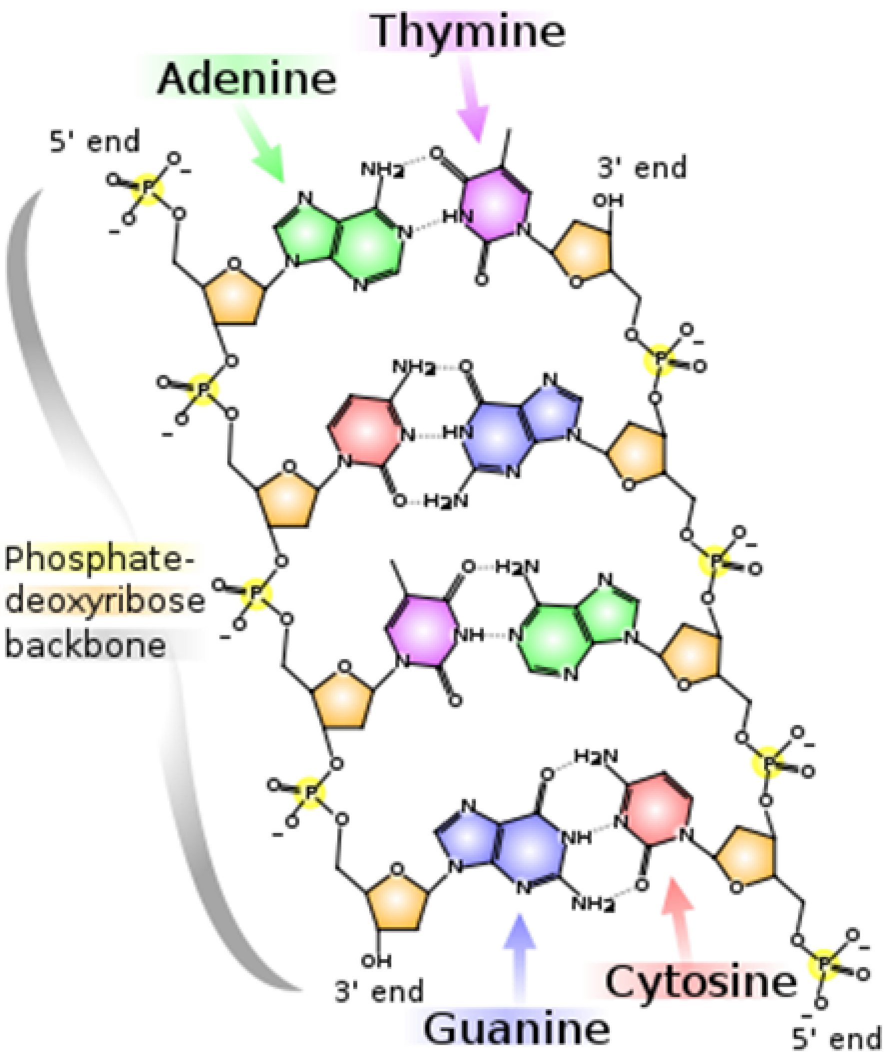
iii) **Response** of living systems to changes of their environment

Not passive, but **ACTIVE**
Complexity of response ~ complexity of the system

Two distinct types of response

- Inherited from ancestors - not modified during life of an individual (HW)
- Modified during life of an individual – process of learning (SW in complex HW)

Deoxyribonucleic Acid (DNA)



4 bases : Adenine **A**
Thymine **T**
Cytosine **C**
Guanine **G**

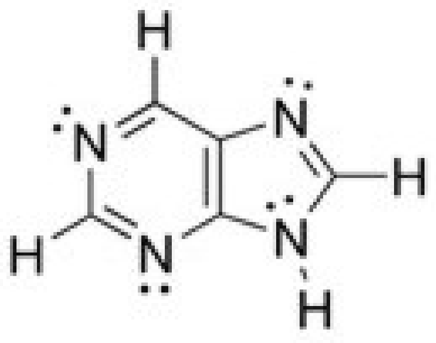
Bound by hydrogen (noncovalent) bonds

A = T, C ≡ G

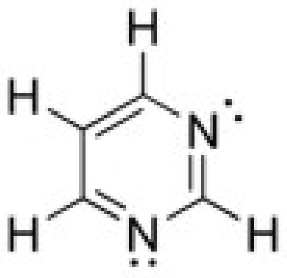
DNA nucleobases

Adenin, Guanine - substituted **purine**
Thymine, Cytosine - substituted **pyrimidine**

Purine



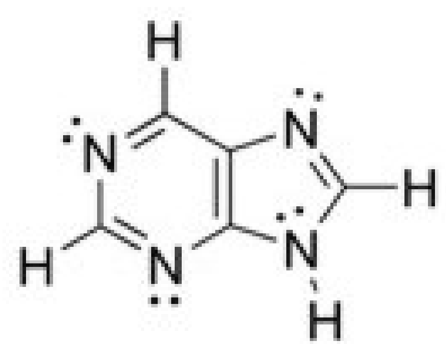
Pyrimidine

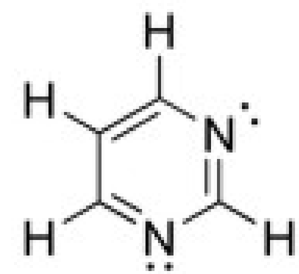


DNA nucleobases

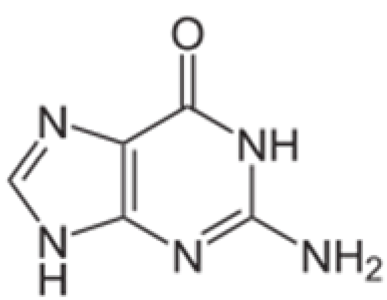
Adenin, Guanine - substituted **purine**
Thymine, Cytosine - substituted **pyrimidine**

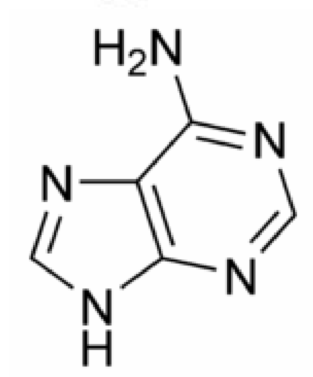
Purine

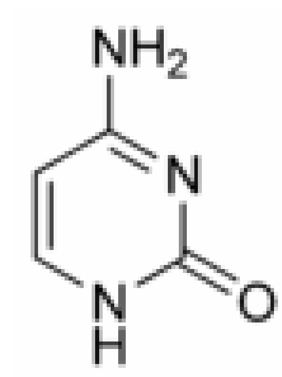


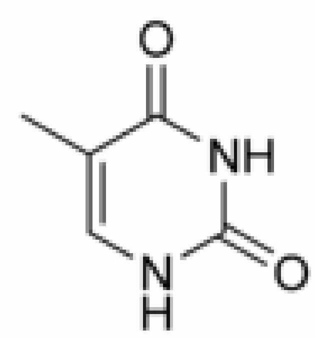


Pyrimidine



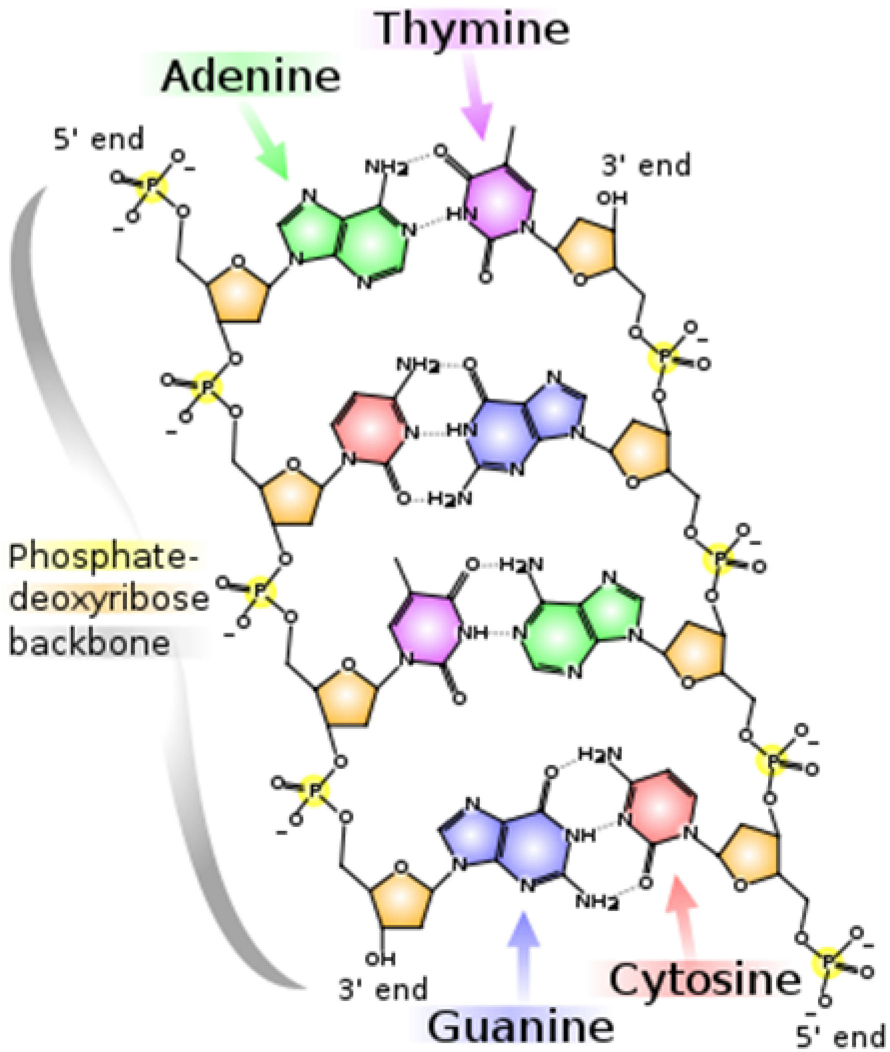


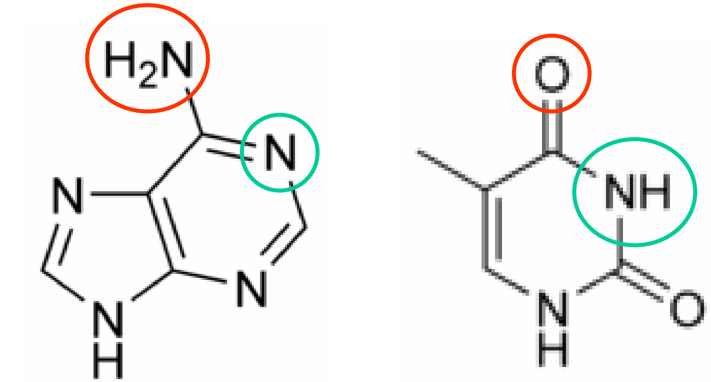




Guanine Adenine Cytosine Thymine

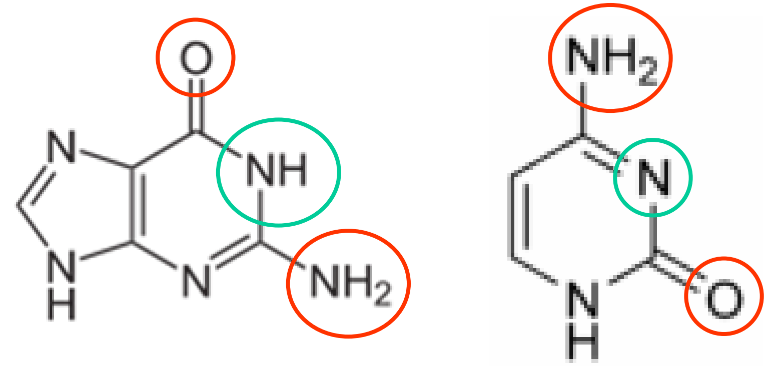
Complementarity of nucleobases



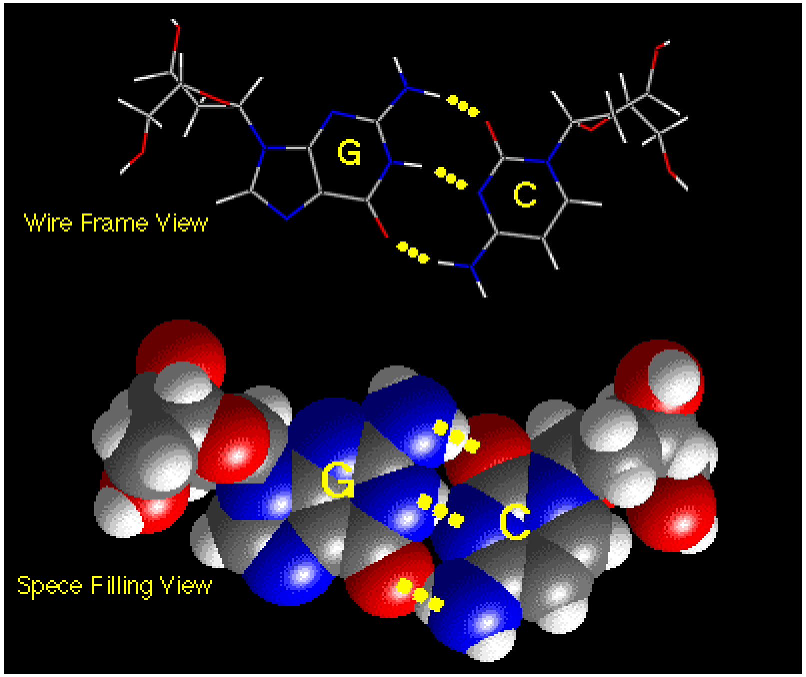


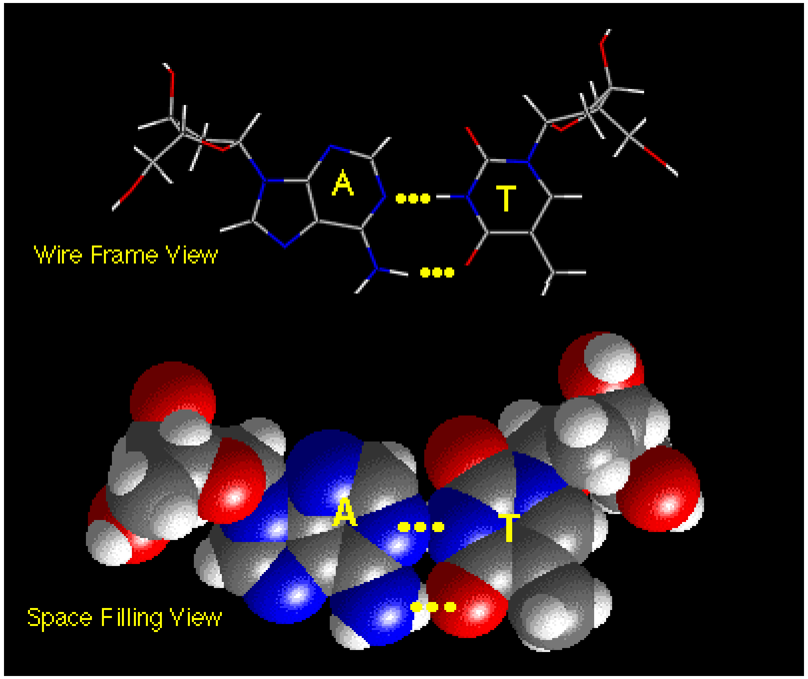
Adenine Thymine

Guanine Cytosine



DNA base pairing



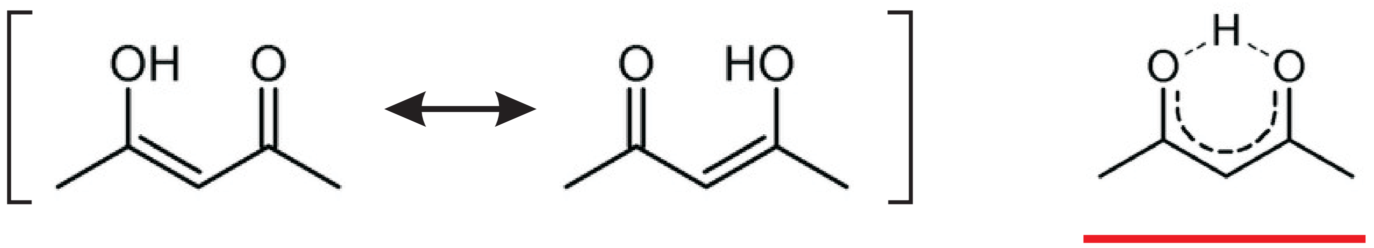


Guanine Cytosine

Adenine Thymine

G-C and A-T are **hydrogen bonds**

Hydrogen bond - intramolecular

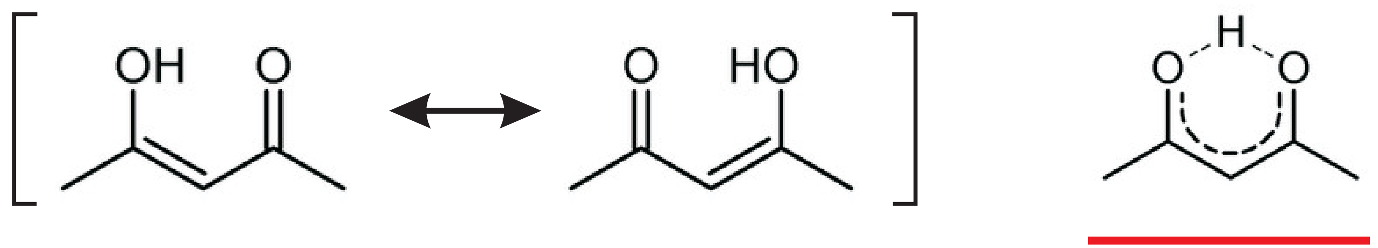


Two structures
(static picture)

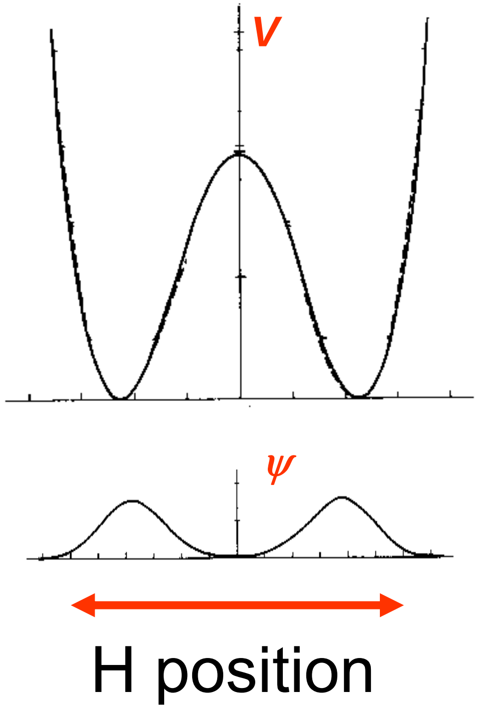
One structure
(dynamic picture)

Specific character – **tunneling** motion (quantum effect)

Hydrogen bond - intramolecular



Tunneling between two structures ~ two minima on the potential energy hypersurface

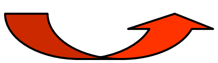


Hydrogen bond - intermolecular

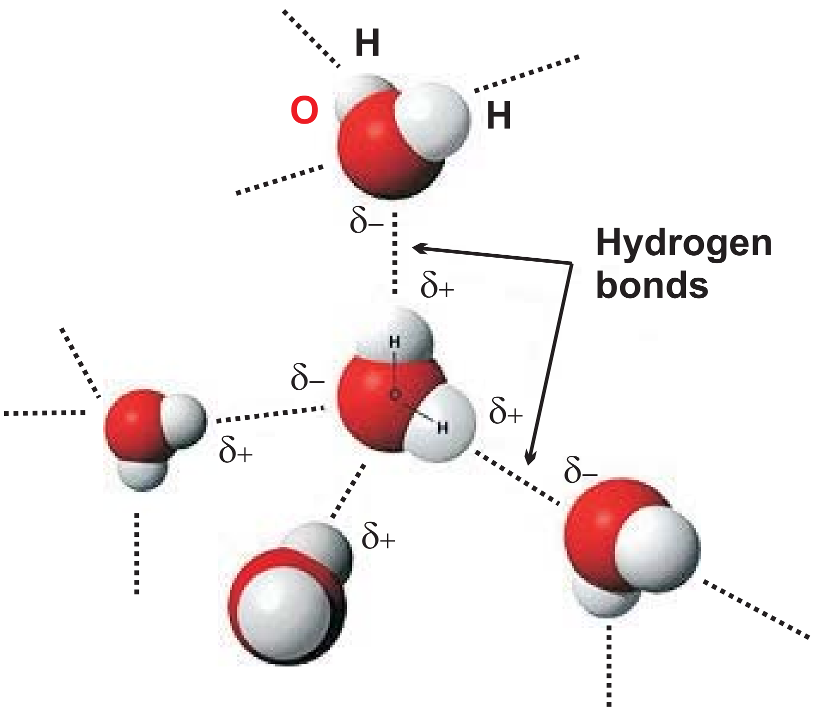
Electrons are more attracted to the more electronegative oxygen than to hydrogen
⇒ partial charges δ+ / δ-

Electrostatic forces
⇒ orientation of molecules

+ Tunneling of H^+
$H_2O + H_2O \leftrightarrow H_3O^+ + OH^-$



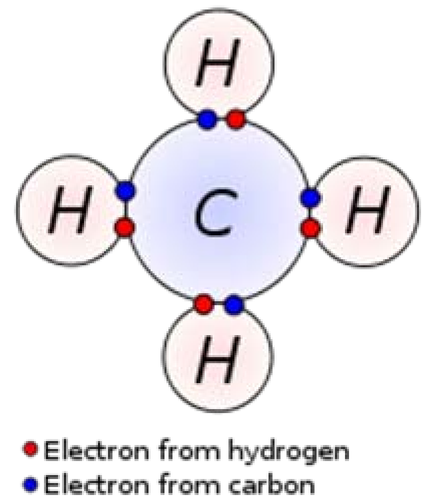
H^+



H_2O – extremely polar ⇒ liquid at temperature 273-373 K
x N_2 63-77 K, H_2 at 14-20 K

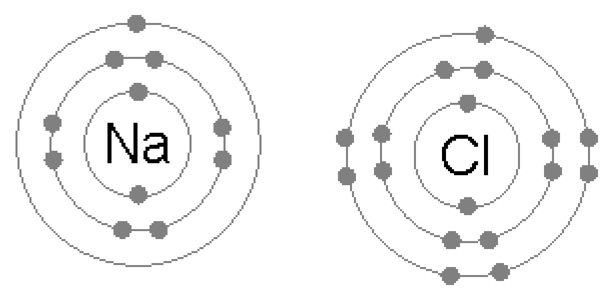
Intermolecular hydrogen bonds

Hydrogen bonds
significantly weaker (~ 5-30 kJ/mol)

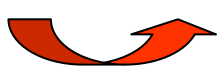


- **Covalent bonds** (intermediated by a shared pair of electrons) ~ 440 kJ/mol

- **Ionic bonds** (complete transfer of an electron, ~750 kJ/mol)



$$\mathrm{Na + Cl + En_1 \rightarrow Na^+ + Cl^- + En_2}$$



e^-

$En_1 < En_2$

Intermolecular hydrogen bonds

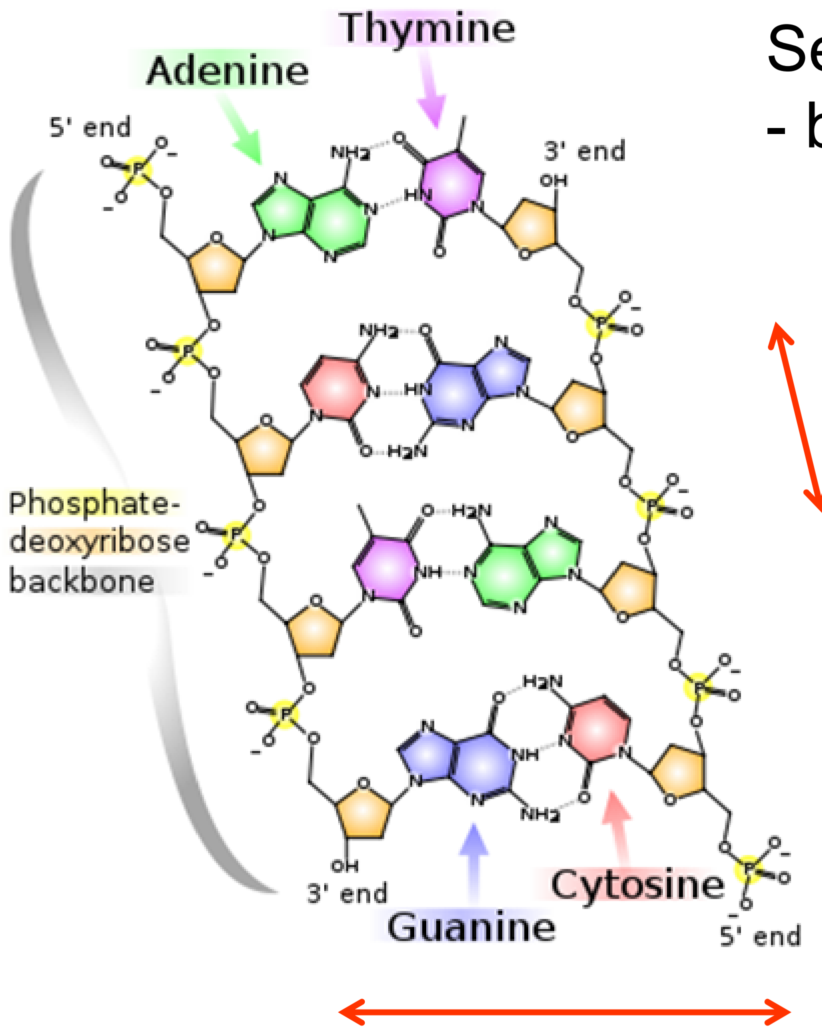
Hydrogen bonds (~ 5-30 kJ/mol)
still stronger than

van der Walls bonds (no shared electrons)
- permanent dipole – permanent dipole (~ 0.5-2 kJ/mol)
- permanent dipole – induced dipole (< 1 kJ/mol)
- induced dipole – induced dipole

Typical properties of bonds

	Bond length (nm)	Energy (kJ/mol)	T (K)
Covalent / Ionic	0.1 – 0.15	150 - 900	500 - 1000
Hydrogen	0.2 – 0.35	5 - 35	300
van der Waals	0.3 – 0.5	0.1 - 2	<100

DNA – typical dimensions



Secondary structure
- base pairing

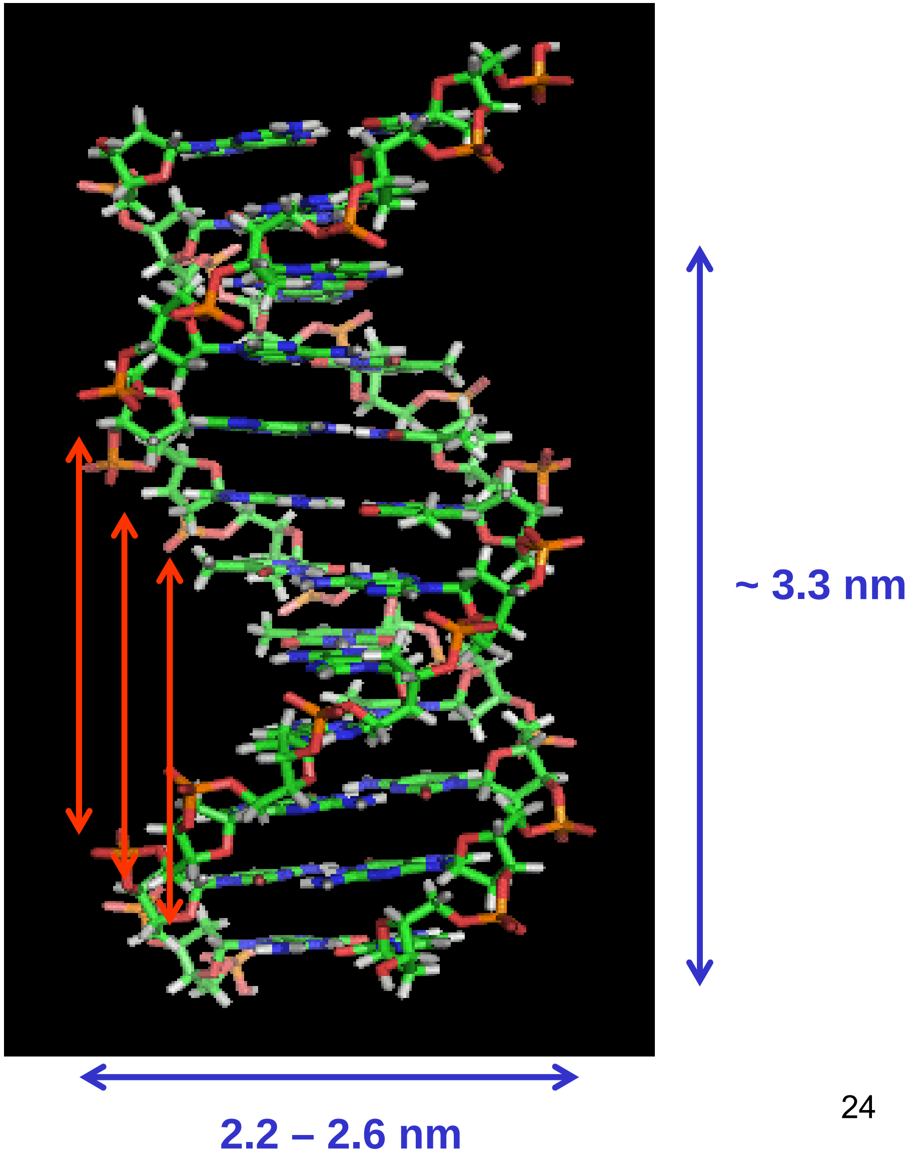
~ 0.33 nm

2.2 – 2.6 nm

DNA structure

Tertiary structure
- spatial, double helix

Stability enhanced by stacking interactions
+ hydration in cells



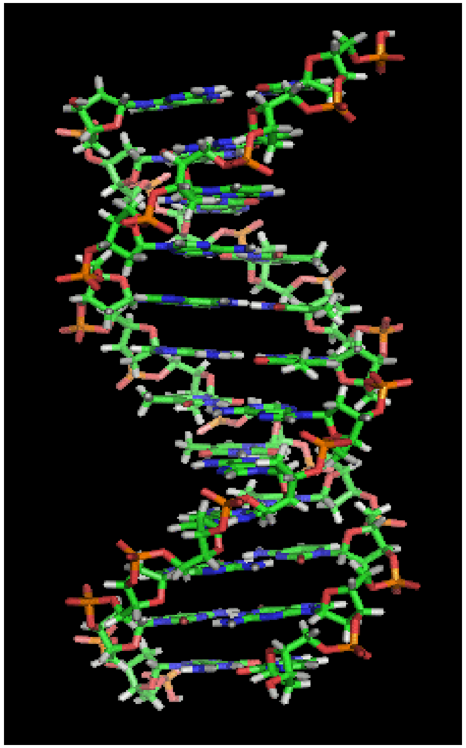
Human DNA

About 3 billion base pairs in the nucleus of each cell
Typical size of a bilogical cell ~ 10^{-5} m (10 μm)
DNA (macro)molecule **~ 1 m long**, ~ 6.10^{-12} g
Only about 1.5 % used for and transfer of genetic information and protein coding (exons)

Number of cells in the human body ~ **10^{13} - 10^{14}**
Unbelievable length of all human DNA molecules

DNA – protein coding

The specific sequences of bases are used for assembling proteins



Transcription of the genetic information to RNA (oxyribonucleic acid) on which the protein is synthesized (translation)

RNA – single strand, thymine → uracil

Proteins – polypeptides built from aminoacids (peptide bonds)
3 DNA/RNA bases code one aminoacid
Typical length of peptides ~ order of 100 aminoacids

Information processing in living systems

Enormous complexity of living matter vs. extremely specific underlying chemical structures - are a manifestation of use of information stored in DNA

Regarded as a process of retrieval of this information and using it in building and functions of living bodies raises many non-trivial questions

Relation between the existence of an information database (DNA) and its emergence

$\Rightarrow$ the ‘chicken or the egg’ dilemma

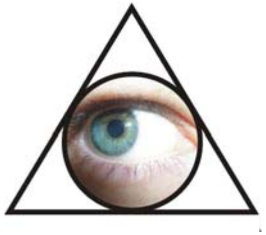
Characteristics of living systems

Where is the boundary between living systems (LS) and lifeless nature?

Analyzing the assembly of complex (living) systems to the simplest constituents $\rightarrow$ self-assembly

The role of information in living systems ?

Do we need some higher-level 'principle' for the initial step ?



Different Concept of Space and Time

Self-assembly of bound systems

Extension of the model to complex systems with properties attributed to ‘living systems’

Modification of the concept of **space** and **time** in the sense that these do not exist independently from bodies, their building blocks, and fields that make them mutually interact, but are inseparable, emergent

Ambitious project for treating **qualitative** changes

Notion of Time

Time is a fundamental physical quantity (~ mass, distance), i.e. it cannot be derived from other fundamental ones (~ velocity = distance / time)

Two distinct viewpoints on time

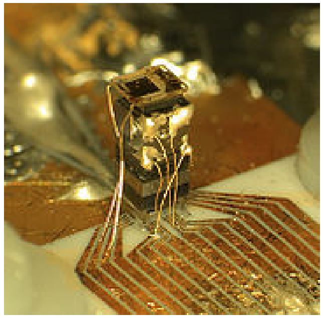
- Time - part of the fundamental structure of the universe, a dimension in which events occur in a sequence
  $\Rightarrow$ Newtonian, relativistic time
- Time does not refer to any ‘frame’ through which objects move and in which events occur, only a kind of intellectual structure (together with space and numbers) in which humans sequence and compare objects and events

Measurements of Time

Need of **linear** and **cyclic** time

Cyclic time = **periodic** process providing a **unit of time**
the simplest unit – day ⇐ observation of the Sun position



Measurements of Time

Need of **linear** and **cyclic** time

Cyclic time = **periodic** process providing a **unit of time**
the simplest unit – day ⇐ observation of the Sun position

Linear time = division of the **periodic** time into equal smaller units

Time measurement – counting ‘clicks’ of the periodic process

Synchronization of **linear** and **cyclic** time

Measurements of Time

Synchronization of linear and cyclic time – not a major issue when there is no interaction between the two 'clocks'

'No interaction' historically meant visual control
But synchronization has to be controlled always by some kind of signal (light) which may affect the periodic motion of the system providing the unit period

Atomic clock – based on quantum transition with a fixed frequency $\Rightarrow$ counting the clicks of the emitted radiation

The second is the duration of 9,192,631,770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the cesium 133 atom.

Measurements of Time

The second is the duration of 9,192,631,770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the cesium 133 atom.

Atomic clock – still represents a lower limit of the **cyclic** time for practical measurements

Space, Time, and Numbers

- **?** Is not the main obstacle to consistent description of quantitative and qualitative changes on one common footing the continuous character of space and time?

- **?** Some principle of ‘least possible’ change in the concept of finite geometries that would imply a least possible change in time and space in the sense that :

- ➢ **Both space and time** only **emerge** at a certain level of complexity of finite geometry objects

- ➢ **All fundamental physical quantities** only **emerge** at a certain level of complexity of finite geometry objects

Space, Time, and Information

- Existence of objects and their interactions would not have to be assumed as primary, but they would also emerge together with **space** and **time**
- Finite geometry approach – a fundamental concept for representing **information** on a common footing with physical objects and interactions?
- Finite geometry – potential language of emergence?

Continuation

Examples of physical problems with emphasis on hierarchic issues