BE564

Biophysics of Large Molecules

Instructor: Maxim Frank-Kamenetskii

Course syllabus, fall 2017

1. *Introduction.* Role of large molecules in biomedical engineering, molecular biology and biotechnology. Polyatomic molecules. Macromolecules. Examples: formaldehyde, benzene, polyethylene, polyacethylene, natural and arificial chromophores and fluorophores, proteins, DNA, RNA.

2. *Basic principles of classical physics*. Symmetry of the space-time and conservation laws. Newton laws. Classical harmonic oscillator. Failure of classical physics to describe atoms and molecules. Triumph of modern (quantum) physics.

3. *Basic principles of quantum physics.* Operators and wavefunctions. Schrödinger equation. Free particle. De Broglie waves of matter. Particle-wave duality. Heisenberg's uncertainty principle. A particle in a stationary external field. Spectrum of states. Harmonic oscillator. A particle in a box. Matrix elements. An electron in the Coulomb potential. Atomic orbitals. Pauli principle. Electronic structure of main "biological" elements: hydrogen, carbon, nitrogen and oxygen. Molecular orbitals. Hybridization. Covalent bonds. σ- and π- bonds.

4. *Polyatomic molecules*. Electronic and nuclear motions. Schrödinger equation for the molecule. Born-Oppenheimer (adiabatic) approximation. The Born-Oppenheimer parameter and its significance. Electronic terms. Nuclear vibrations. Normal modes. Zero-point vibrations. Ground and excited states. Time-dependent Schrödinger equation. Transitions between different states.

5. *Molecular photonics: its role in biology and biotechnology.* Photon absorption. The Beer-Lambert law. Transition probabilities. Electronic and vibrational spectra of polyatomic molecules. Selection rules. Singlet and triplet electronic terms. Luminescence, fluorescence and phosphorescence. Radiationless transitions. Excitation lifetime. Chromophores and fluorophores in biology and biotechnology. Fluorescent microscopy. The Abbe limit. Super-resolved fluorescence microscopy. Molecular mechanisms of vision: retinal and rhodopsin. Channelrhodopsin and advent of optogenetics; neuroscience revolution. Green fluorescent protein (GFP) and its analogs. Dyes and quantum dots and their role in biotechnology. Fluorescence resonance energy transfer (FRET). Molecular beacons and Real Time PCR.

6. *Group theory.* Group definition. Examples: digits, braids, symmetry operations, matrices, fundamental group, knot group. The representation theory. Reducible and irreducible representations. Characters.

7. *Molecular symmetry.* Symmetry groups and their representations. Example: formaldehyde.

Classifications of electronic terms. Classification of normal modes. Selection rules. Symmetry forbidden transitions. Electronic and vibrational spectra of benzene.

8. *Basic principles of statistical physics.* Thermal motion and thermal equilibrium. Brownian motion. Energy and entropy. Gibbs distribution. Partition function. Classical statistical mechanics. Equipartition theorem. Quantum statistics: photons and phonons. Blackbody radiation. Planck's equation. Wien law. Heat capacity of solids. Debye theory. Role of statistical mechanics in understanding the behavior of polyatomic molecules and macromolecules.

9. *Macromolecules.* Role of the carbon atom. Polymerization and polycondensation. The nature of flexibility of the polymer chain. Theoretical models of polymers. Freely-Jointed Chain (FJC). Mean-square end-to-end distance. Kuhn statistical length. Worm-Like Chain (WLC). Persistence length. DNA as a macromolecule. Analogy between the bodiless polymer chain and Brownian motion. Polymeric coil. Role of entropy. Distribution function for the end-to-end distance for FJC. High elasticity. Nature of high elasticity.

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Textbooks:

1. I.Tinoco, et al. *Physical Chemistry*: *Principles and Applications in Biological Sciences.* 5th edition, Pearson Education, Inc. USA, 2014. https://www.amazon.com/Physical-Chemistry-Principles-Applications-Biological/dp/0136056067/ref=sr_1_fkmr0_1?s=books&ie=UTF8&qid=1474564082&sr=1-1-fkmr0&keywords=I.Tinoco+physical+chemistry+biology+applications
2. N.Dalarsson et al. *Introductory Statistical Thermodynamics.* Academic Press, Amsterdam, etc., 2011 https://www.amazon.com/Introductory-Statistical-Thermodynamics-Engineering-Mathematical/dp/012384956X/ref=sr_1_3?s=books&ie=UTF8&qid=1472156833&sr=1-3&keywords=Dalarsson
3. R.M. Hochstrasser Molecular Aspects of Symmetry. W.A.Benjamin, Inc. New York & Amsterdam, 1966. https://www.amazon.com/Molecular-Aspects-Symmetry-Robin-Hochstrasser/dp/B0006BNW5I/ref=sr_1_1?s=books&ie=UTF8&qid=1472157088&sr=1-1&keywords=molecular+aspects+of+symmetry