Biophysics and chemical physics

Coordinated by: Institute of Physics Charles University
Study programme coordinator: prof. RNDr. Marek Procházka, Ph.D.

Characterization of the study program:

The focus of this field lies at the interface of physics, biology and chemistry. The study program builds on basic physical education, which deepens in the areas of theoretical and experimental physics important for the description and research of molecules, biopolymers, supramolecular systems and biological objects. The graduate will gain knowledge of quantum theory and statistical physics of molecules and molecular systems, experimental methods of biophysics and chemical physics, especially optical and other spectroscopic methods, structural analysis and imaging techniques. Students choose one of two specializations: theoretical or experimental biophysics and chemical physics. In the theoretical specialization they will gain deeper knowledge in the field of quantum chemistry, molecular dynamics or advanced theoretical spectroscopy; in experimental in the field of biochemistry and molecular biology, biophysics of photosynthesis or structural methods. Through regular seminars, diploma theses, and thematically focused lectures, students gain an idea of current problems addressed in various fields and methods of scientific work. Thanks to a wide range of knowledge, graduates have the opportunity to apply in research and applied fields related to physics, biology, chemistry, medicine, materials research, bio- and nano-technologies, pharmacy, etc.

Profile of the graduates and aims of the study:

The graduate knows quantum theory and statistical physics of molecules and molecular systems, experimental methods of biophysics and chemical physics, especially optical and other spectroscopic methods, structural analysis and imaging techniques. Graduates of the theoretical specialization will gain deeper knowledge in the field of quantum chemistry, molecular dynamics or advanced theoretical spectroscopy. Graduates of the experimental specialization will gain deeper knowledge in the field of biochemistry and molecular biology, biophysics of photosynthesis or structural methods. Through regular seminars, students will gain an idea of current problems addressed in various fields and methods of scientific work. They are proficient in communicating professional knowledge in the form of presentations or written texts, also in English. Some graduates are expected to pursue a career as a researcher. The acquired education also offers graduates employment in interdisciplinary teams dealing with physics, biology, chemistry, medicine, materials research, bio- and nano-technologies or pharmacy.

Recommended plan of the study

The field offers students two specializations - experimental and theoretical. Students usually select a specialization after the end of the first semester (1st year of Mgr. Studies, winter semester). Until then, the courses of study in both specializations are the same.

Within each specialization, students have the opportunity for a further narrower focus of their study, which will be reflected in the choice of questions for the final state examination. Students choose two thematic areas (from three possible) and to the courses from compulsory optional courses of group I. In experimental specialization, these are areas: 1. Biochemistry and molecular biology (courses NBCM012, NBCM008), 2. Optical spectroscopy and biophysics of photosynthesis (courses NBCM179, NBCM088) and

3. Structural methods (courses NBCM098, NBCM112). In theoretical specialization, these are areas: 1. Quantum chemistry (courses NBCM121, NBCM122, NBCM155), 2. Molecular dynamics and statistics (courses NBCM346, NBCM100, NFPL004) and 3. Advanced theoretical spectroscopy (courses NBCM154, NBCM027, NOOE119).

A pre-requisite of the study in this program is knowledge of quantum theory and general chemistry on the Bachelor level.

Specialization: Experimental biophysics and chemical physics

Compulsory and compulsory-optional courses – group I (25 credits)

First year of the Master study

Code	Subject	Credits	Winter	Summer
NBCM010	**Bioorganic chemistry**	4	2/1 C+Ex	—
NBCM177	**Experimental methods of biophysics and chemical physics I**	6	4/0 Ex	—
NBCM160	**Classical and quantum statistical physics of molecular systems**	4	3/0 Ex	—
NBCM039	**Quantum Theory of Molecules**	7	3/2 C+Ex	—
NBCM095	**Practical Course in Experimental Methods of Biophysics and Chemical Physics I**	7	0/5 MC	—
NSZZ023	**Diploma Thesis I**	6	—	0/4 C
NBCM178	**Experimental methods of biophysics and chemical physics II**	3	—	2/0 Ex
NBCM088	Biophysics of Photosynthesis	3	—	2/0 Ex
NBCM012	Biochemistry	4	—	3/0 Ex
NBCM112	Magnetic Resonance Methods in Biophysics	4	—	3/0 Ex
NBCM179	Advanced methods of optical spectroscopy	4	—	3/0 Ex
NBCM103	Practical Course in Experimental Methods of Biophysics and Chemical Physics II	7	—	0/5 MC

Second year of the Master study

Code	Subject	Credits	Winter	Summer
NSZZ024	**Diploma Thesis II**	9	0/6 C	—
NBCM175	**Seminar of biophysics and chemical physics I**	3	0/2 C	—
NSZZ025	**Diploma Thesis III**	15	—	0/10 C
NBCM176	**Seminar of biophysics and chemical physics II**	3	—	0/2 C

NBCM008	Molecular and Cell Biology for Biophysicist	4	3/0 Ex	—
NBCM098	X-ray and Electron Structure Analysis of Biomolecules and Macromolecules	3	2/0 Ex	—
NBCM165	Theoretical bases of molecular spectroscopy	3	2/0 Ex	—

Compulsory-optional courses – group II (15 credits)

Code	Subject	Credits	Winter	Summer
NBCM101	Detection and Spectroscopy of Single Molecules	3	2/0 Ex	—
NBCM033	Physical Principles of Photosynthesis	3	2/0 Ex	—
NFPL185	Advanced High Resolution NMR Spectroscopy	5	2/1 C+Ex	—
NBCM158	Practical aspects of experimental data treatment	3	1/1 Ex	—
NBCM014	Structure, Dynamics and Functions of Biomembranes	3	2/0 Ex	—
NBCM023	Importance and Functions of Metal Ions in Biological Systems	3	2/0 Ex	—
NBCM102	Fundamentals of Classical Radiometry and Photometry	3	2/0 Ex	—
NBCM026	Experimental Technology in Molecular Spectroscopy	3	—	2/0 Ex
NFPL179	Quantum Description of NMR	5	—	2/1 C+Ex
NBCM114	Optical Microscopy and Selected Imaging Techniques in Biophysics	3	—	2/0 Ex
NOOE012	Scattering Methods in Optical Spectroscopy	3	—	2/0 Ex
NBCM097	Surface-Enhanced Raman Spectroscopy	3	—	2/0 Ex
NBCM172	Two-dimensional electronic spectroscopy	3	1/1 C+Ex	1/1 C+Ex
NBCM316	Computer Modelling of Biomolecules	4	1/2 C+Ex	1/2 C+Ex
NBCM018	One-week Practical Course in Biochemistry	3	0/2 C	0/2 C

Recommended optional courses

Code	Subject	Credits	Winter	Summer
NBCM121	*Ab Initio Methods and Density Functional Theory I*	5	—	2/1 C+Ex

NBCM122	*Ab Initio Methods and Density Functional Theory II*	3	2/0 Ex	—
NBCM173	*Ab-initio methods for periodic systems*	3	2/0 Ex	—
NBCM307	*Astrobiology*	3	2/1 Ex	—
NBCM024	*Yeast Biology*	3	—	2/0 Ex
NBCM150	*Physical observation of nano-objects*	5	2/1 C+Ex	2/1 C+Ex
NAFY018	*Chemistry for Physicists*	4	2/1 C+Ex	—
NBCM106	*Chemistry for Physicists II — Analytical Chemistry*	6	—	2/2 C+Ex
NBCM156	*Chiroptic spectroscopy*	3	—	2/0 Ex
NBCM154	*Quantum electrodynamics*	3	—	2/0 Ex
NBCM134	*Quantum Theory of Resonances*	3	—	2/0 Ex
NBCM051	*Molecular Dynamics and Monte Carlo Methods*	5	2/1 C+Ex	—
NBCM346	*Molecular dynamics I*	5	—	2/1 C+Ex
NBCM347	*Molecular dynamics II*	5	2/1 C+Ex	—
NBCM181	*Molecular dynamics — calculations of free energy*	3	1/2 MC	1/2 MC
NBCM055	*Molecular Simulations for solving of material structure*	5	2/1 C+Ex	2/1 C+Ex
NBCM149	*Nanotechnology in biology*	3	2/0 C	2/0 C
NOOE119	*Nonlinear Optical Spectroscopy*	3	—	2/0 Ex
NFPL004	*Nonequilibrium Statistical Physics and Thermodynamics*	3	2/0 Ex	—
NBCM305	*Optical Sensors*	3	2/0 Ex	—
NBCM099	*Practical Exercises in Quantum Theory of Molecules I*	4	—	0/3 C
NBCM116	*Practical Exercises in Quantum Theory of Molecules II*	4	0/3 C	—
NAFY080	*Preparation of Biological Samples*	3	—	2/0 Ex
NOOE015	*Seminar*	2	—	0/1 C
NFPL186	*Seminar on High Resolution NMR Spectroscopy*	3	0/2 C	0/2 C
NBCM027	*Symmetry of Molecules*	4	—	2/1 C+Ex
NFPL003	*Synthetic Problems of Quantum Theory*	3	—	2/0 C
NBCM115	*Scientific Photography and Related Imaging Techniques*	3	1/1 Ex	—
NPRF005	*UNIX and LINUX for Physicists*	3	2/0 C	—
NBCM159	*Introduction to Computer Control of Experiment*	4	—	1/2 MC
NBCM308	*Introduction to Protein Structure Studies*	3	—	2/0 Ex
NBCM100	*Computational Experiments in Molecular Theory I*	4	—	0/3 MC

NBCM125	*Computational Experiments in Molecular Theory II*	6	—	0/4 MC
NBCM041	*Fundamentals of Energy Transfer in Molecular Systems I*	3	2/0 Ex	—

Specialization: Theoretical biophysics and chemical physics

Compulsory and compulsory-optional courses – group I (25 credits)

First year of the of the Master study

Code	Subject	Credits	Winter	Summer
NBCM010	**Bioorganic chemistry**	4	2/1 C+Ex	—
NBCM177	**Experimental methods of biophysics and chemical physics I**	6	4/0 Ex	—
NBCM160	**Classical and quantum statistical physics of molecular systems**	4	3/0 Ex	—
NBCM039	**Quantum Theory of Molecules**	7	3/2 C+Ex	—
NBCM095	**Practical Course in Experimental Methods of Biophysics and Chemical Physics I**	7	0/5 MC	—
NSZZ023	**Diploma Thesis I**	6	—	0/4 C
NBCM178	**Experimental methods of biophysics and chemical physics II**	3	—	2/0 Ex
NBCM121	Ab Initio Methods and Density Functional Theory I	5	—	2/1 C+Ex
NBCM154	Quantum electrodynamics	3	—	2/0 Ex
NBCM346	Molecular dynamics I	5	—	2/1 C+Ex
NBCM100	Computational Experiments in Molecular Theory I	4	—	0/3 MC

Second year of the of the Master study

Code	Subject	Credits	Winter	Summer
NSZZ024	**Diploma Thesis II**	9	0/6 C	—
NBCM175	**Seminar of biophysics and chemical physics I**	3	0/2 C	—
NSZZ025	**Diploma Thesis III**	15	—	0/10 C
NBCM176	**Seminar of biophysics and chemical physics II**	3	—	0/2 C
NBCM122	Ab Initio Methods and Density Functional Theory II	3	2/0 Ex	—
NBCM155	Field theory methods in the theory of many particles	3	2/0 Ex	—

NFPL004	Nonequilibrium Statistical Physics and Thermodynamics	3	2/0 Ex	—
NBCM027	Symmetry of Molecules	4	—	2/1 C+Ex
NBCM165	Theoretical bases of molecular spectroscopy	3	2/0 Ex	—
NOOE119	Nonlinear Optical Spectroscopy	3	—	2/0 Ex

Compulsory-optional courses – group II (15 credits)

Code	Subject	Credits	Winter	Summer
NBCM067	Quantum Optics I	5	2/1 C+Ex	—
NBCM347	Molecular dynamics II	5	2/1 C+Ex	—
NBCM131	Advanced Methods in Molecular Dynamics	3	2/0 Ex	—
NBCM041	Fundamentals of Energy Transfer in Molecular Systems I	3	2/0 Ex	—
NBCM093	Quantum Optics II	5	—	2/1 C+Ex
NBCM134	Quantum Theory of Resonances	3	—	2/0 Ex
NBCM099	Practical Exercises in Quantum Theory of Molecules I	4	—	0/3 C
NBCM116	Practical Exercises in Quantum Theory of Molecules II	4	0/3 C	—
NBCM125	Computational Experiments in Molecular Theory II	6	—	0/4 MC
NBCM055	Molecular Simulations for solving of material structure	5	2/1 C+Ex	2/1 C+Ex
NBCM180	Theoretical seminar of biophysics and chemical physics	4	0/1 C	0/1 C

Recommended optional courses

Code	Subject	Credits	Winter	Summer
NBCM173	*Ab-initio methods for periodic systems*	3	2/0 Ex	—
NBCM307	*Astrobiology*	3	2/1 Ex	—
NBCM184	*Asymptotic Methods in Physics*	5	2/1 C+Ex	—
NBCM088	*Biophysics of Photosynthesis*	3	—	2/0 Ex
NBCM012	*Biochemistry*	4	—	3/0 Ex
NBCM101	*Detection and Spectroscopy of Single Molecules*	3	2/0 Ex	—
NBCM172	*Two-dimensional electronic spectroscopy*	3	1/1 C+Ex	1/1 C+Ex
NBCM026	*Experimental Technology in Molecular Spectroscopy*	3	—	2/0 Ex
NBCM150	*Physical observation of nano-objects*	5	2/1 C+Ex	2/1 C+Ex
NBCM033	*Physical Principles of Photosynthesis*	3	2/0 Ex	—

NBCM156	*Chiroptic spectroscopy*	3	—	2/0 Ex
NBCM067	*Quantum Optics I*	5	2/1 C+Ex	—
NFPL179	*Quantum Description of NMR*	5	—	2/1 C+Ex
NBCM112	*Magnetic Resonance Methods in Biophysics*	4	—	3/0 Ex
NBCM051	*Molecular Dynamics and Monte Carlo Methods*	5	2/1 C+Ex	—
NBCM008	*Molecular and Cell Biology for Biophysicist*	4	3/0 Ex	—
NBCM181	*Molecular dynamics — calculations of free energy*	3	1/2 MC	1/2 MC
NBCM114	*Optical Microscopy and Selected Imaging Techniques in Biophysics*	3	—	2/0 Ex
NBCM316	*Computer Modelling of Biomolecules*	4	1/2 C+Ex	1/2 C+Ex
NTMF002	*Advanced Quantum Theory*	6	3/1 C+Ex	—
NFPL185	*Advanced High Resolution NMR Spectroscopy*	5	2/1 C+Ex	—
NBCM179	*Advanced methods of optical spectroscopy*	4	—	3/0 Ex
NBCM158	*Practical aspects of experimental data treatment*	3	1/1 Ex	—
NBCM103	*Practical Course in Experimental Methods of Biophysics and Chemical Physics II*	7	—	0/5 MC
NBCM098	*X-ray and Electron Structure Analysis of Biomolecules and Macromolecules*	3	2/0 Ex	—
NOOE012	*Scattering Methods in Optical Spectroscopy*	3	—	2/0 Ex
NOOE015	*Seminar*	2	—	0/1 C
NFPL186	*Seminar on High Resolution NMR Spectroscopy*	3	0/2 C	0/2 C
NFPL003	*Synthetic Problems of Quantum Theory*	3	—	2/0 C
NPRF005	*UNIX and LINUX for Physicists*	3	2/0 C	—
NBCM159	*Introduction to Computer Control of Experiment*	4	—	1/2 MC
NBCM308	*Introduction to Protein Structure Studies*	3	—	2/0 Ex
NBCM115	*Scientific Photography and Related Imaging Techniques*	3	1/1 Ex	—
NBCM102	*Fundamentals of Classical Radiometry and Photometry*	3	2/0 Ex	—

NBCM042	*Fundamentals of Energy Transfer in Molecular Systems II*	3	—	2/0 Ex

Conditions that must be satisfied to register for the state final exam

– gain of at least 120 credits
– passing all compulsory courses
– passing the compulsory-optional courses from group I in the extent of at least 25 credits
– passing the compulsory-optional courses from group II in the extent of at least 15 credits
– submission of the completed diploma thesis within the given deadline

Requirements for the oral part of the state final exam

A. Common requirements

1. Quantum theory and statistical physics of molecules and molecular systems (one question in the state exam)

– Antisymmetry of wave function, exchange interaction.
– Born - Oppenheimer and adiabatic approximation.
– Molecule of hydrogen. Atomic and molecular orbitals.
– LCAO method and valence bond method, classification of electron levels, Hückel method.
– One-particle approximation, Hartree and Hartree - Fock equations, Roothan equations.
– Fundamentals of density functional theory, Hohenberg-Kohn theorems.
– Introduction to methods of configuration interaction, bound clusters and perturbation theories, basic equations and properties, Brillouin's theorem.
– Pauli and Dirac equations. Spin-orbital and spin-spin interaction.
– Orbital and spin magnetic moment and their interactions with external fields.
– Quantization of electromagnetic field, interaction of electromagnetic radiation with molecules. Fermi's golden rule.
– Absorption, stimulated and spontaneous emission. Dipole approximation, selection rules.
– Force fields in molecular systems.
– Basic statistical files and distributions, ergodic theorem.
– Monte Carlo method.
– Classical molecular dynamics.
– Liouville's equation.
– Density matrix. Wigner density.
– Basic quantum statistical distributions.
– Evolution of the density matrix (Liouville-von Neumann equation).
– Quantum control of the equation, reduced densities.

2. Experimental methods of biophysics and chemical physics (one question in the state exam)

– Sources, detectors and spectrum analyzers in optical spectroscopy.

- Interaction of optical radiation with an isolated molecule. Selection rules for electronic, vibrational and rotational optical transitions.
- Methods and applications of electron absorption spectroscopy. Excitation and sounding method.
- Methods and applications of vibrational absorption spectroscopy.
- Methods of elastic, dynamic and Brillouin scattering and their use.
- Raman scattering, methods of measurement and use.
- Use of polarized radiation and its analysis in optical spectroscopy. Linear and circular dichroism, emission anisotropy.
- Principles and basic concepts of luminescence (types of luminescence, Jablonsky diagram, kinetics, quantum yield, lifetimes, Franck-Condon principle).
- Influence of intermolecular interactions on luminescence parameters (environmental influence, resonant energy transfer, emission quenching).
- Single-molecular spectroscopy. Influence of interaction with the environment on the shape of the spectral line.
- Measurement of stationary and time-resolved luminescence.
- Scattering and diffraction of X-rays, electrons and neutrons.
- Principles of basic diffraction methods. Symmetry and structure of crystals and their determination from the diffraction pattern.
- Electron microscopy, atomic force microscopy and scanning tunneling microscopy.
- Mass spectrometry.
- Nuclear magnetic resonance: principle, experimental setup, excitation and signal detection, basic pulse sequence.
- High resolution NMR of organic substances in liquids: interpretation of spectra.
- Electron paramagnetic resonance: principle, experimental setup, application.
- Separation methods (centrifugation, chromatography, electrophoresis).

B Specialization Experimental biophysics and chemical physics

The third question of the state exam is chosen from two thematic areas, which the student chooses according to his focus.

1. Biochemistry and molecular biology

- Composition and structure of basic biomolecules (nucleic acids, proteins, carbohydrates).
- Glycolysis and glycolytic reactions. Anaerobic degradation of sugars. Cori cycle.
- Aerobic degradation of sugars. Formation of acetylcoenzyme A.
- The citrate cycle and its amorphous nature. Oxidative phosphorylation.
- Biological membranes, selective permeability of biological membranes, types of transport through the biological membrane.
- Structure of bacterial and eukaryotic cells, cell division, cell cycle.
- DNA arrangement in cells, structure and function of chromosomes, chromatin and nucleosomes, centromere and telomere functions, histones, epigenetic inheritance and prions.
- Genetic information processing, DNA replication, RNA transcription and modification, RNA world, prokaryotic and eukaryotic translation.
- Basic principles of gene expression regulation, prokaryotic and eukaryotic transcription initiation regulation, gene silencing.

– Mutations and mutagenesis, DNA damage and repair of damaged DNA, correction of errors caused by DNA replication.
– Methods of studying DNA and gene expression, genetic engineering, fluorescent proteins.

2. Optical spectroscopy and biophysics of photosynthesis

– Fluorescent labels and probes, fluorescent proteins, protein fluorescence.
– Nonlinear methods of Raman scattering (HRS, SRS, CARS), Raman optical activity (ROA).
– Advanced techniques of Raman spectroscopy (SERS, CRM, DCDR).
– Generation and characterization of femtosecond pulses. Fundamentals of 2DES spectroscopy.
– Nonlinear optical phenomena and their use in optical spectroscopy.
– High spectral resolution methods. Low temperature spectroscopy.
– Transmission and quenching of excitation in photosynthetic antennas.
– Charge distribution and transfer in low- and high-potential reaction centers.
– Electron transfer through the photosynthetic membrane, phosphorylation, comparison with the respiratory membrane.
– Carbon fixation in photosynthesis.
– Biophysical methods of examination and measurement of photosynthesis (variable fluorescence, gasometry, photoacoustic spectroscopy).

3. Structural methods

– Temperature oscillations and their influence on diffraction recording. Patterson's function and its use in solving crystal structures.
– Methods for solving the phase problem of structural analysis.
– Structural factor and Friedel's law. Preferred orientation of crystallites - texture.
– Comparison, construction and use of transmission and scanning electron microscopes.
– Principles and principles of preparation of preparations for TEM and SEM. Mechanism of image formation in TEM and SEM
– Electric and magnetic moments of atomic nuclei, energy in electric and magnetic fields, the phenomenon of nuclear magnetic resonance. Nuclear paramagnetism, relaxation processes.
– High resolution NMR spectroscopy in liquid and solid phase: spin Hamiltonian, types of interactions and their manifestations in spectra, high resolution methods in solid phase.
– One- and multidimensional pulse NMR: concept, basic pulse sequences, use of coherent polarization transfer and nuclear Overhauser effect.
– MR imaging: instrumentation, the principle of achieving spatial resolution, methods of contrast, special applications (angiography, fMRI, MRI spectroscopy).
– Electron spin (paramagnetic) resonance: continuous and pulse methodology of experiment, spin Hamiltonian, interactions and their manifestations in spectra.

B Specialization Theoretical biophysics and chemical physics

The third question of the state exam is chosen from two thematic areas, which the student chooses according to his focus.

1. *Quantum chemistry*
   - Comparison of restricted and unrestricted Hartree-Fock equations and their properties.
   - Configuration interaction methods, formulation and characteristics.
   - Application of perturbation theory to the calculation of correlation energy, Møller-Plesset method.
   - Bound cluster method, excitation operators, equations and basic properties.
   - Conceptual theory of density functional - chemical potential, hardness and softness of electron density, Fukui function; time-dependent theory.
   - Weak intermolecular interactions; multipole approximation.
2. *Molecular dynamics and statistics*
   - Numerical propagators derived from the Liouville operator.
   - Algorithms for pressure control, temperature control algorithms. Fixation and restriction of degrees of freedom.
   - Non-equilibrium molecular dynamics.
   - Molecular mechanics, parameterization of force fields.
   - Methods of molecular simulations – counting of non-binding interactions, analysis of trajectories.
   - Stochastic processes (Langevin dynamics, normal and anomalous diffusion).
   - Stochastic quantum dynamics.
   - Entropy in nonequilibrium processes (Boltzmann's H-, Jarzynski and fluctuation theorems).
3. *Advanced theoretical spectroscopy*
   - Symmetry in quantum mechanics (quantum numbers, block diagonalization of Hamiltonian).
   - Symmetry in the spectroscopy of atoms and molecules (selection rules, allowed and forbidden transitions, reduction of symmetry in external electromagnetic fields).
   - Scattering of photons on an atom (Rayleigh, Raman, resonant and Thomson scattering).
   - Radiation correction to atomic spectra (Lamb's displacement, natural energy of electron and photon).
   - The shape of the absorption line (linear response theory, correlation function of the bath).
   - Perturbation theory for time-resolved nonlinear spectroscopy (excitation and probing method, photon echo).