PhD topics in EN study programmes at Faculty of chemistry BUT for the 2022

Topic: **Non-equilibrium thermodynamics and the theory of chemical kinetics**

Supervisor: [Pekař Miloslav, prof. Ing., CSc.](https://www.fch.vut.cz/lide/pekar-miloslav-2035)

**Study program: Physical Chemistry**

The results, which have been obtained within the area of macroscopic non-equilibrium thermodynamics, show tighter links between chemical thermodynamics and kinetics than usually supposed. Thermodynamics delineates the general framework which determines, among other, also the form of rate equations and puts some restrictions on coefficients occurring in these equations. The corresponding thermodynamic theory has been elaborated only for the linear fluids to date and even here some interesting questions remain to be answered. During this PhD study, following problems will be solved successively:

• kinetics in non-ideal fluid mixtures, applicability of activity in kinetic equations;

• application of the thermodynamic theory on reaction mechanisms with activated complex, study of relationships to the corresponding microscopic theory (of activated complex) and to the preceding problem;

• application of the theory on several selected published mechanisms, comparison of thus obtained kinetic equations with the published equations, discussion of the contribution of the novel theory to the praxis of reaction kinetics;

• extension of the theory outside the linear fluid model, focused particularly on reacting systems with significant effect of diffusion and on the relationship between the rate of reaction and diffusion.

Topic: **Advanced materials for organic photonics**

Supervisor: [doc. Mgr. Martin Vala, Ph.D.](https://www.fch.vut.cz/en/people/martin-vala-50351)

**Study program: Physical Chemistry**

Advanced organic materials represent a very interesting alternative to traditional inorganic substances used in photonic applications. Organic materials provide a number of potential advantages such as flexibility, low weight, preparation with low-cost material printing techniques, wide range of parameter tuning, low environmental impact, etc.

This work will deal with the study of the relationship between (especially) optical properties and the chemical structure of organic pi-conjugated molecules (dyes, pigments). One of the target applications will be organic solid-state lasers. Part of the work will be the preparation and study of such model structures. In particular, properties related to radiative and non-radiative processes after photoexcitation will be studied. Typical methods of study will include absorption and fluorescence spectroscopy, determination of fluorescence lifetime and quantum yields, and determination of threshold excitation energy to induce amplified spontaneous emission (ASE) and other parameters affecting their function.

The work will take place within the Laboratory of Organic Electronics and Photonics (https://www.fch.vut.cz/vav/cmv/laboratore/elektro) at the Center for Materials Research at the Faculty of Chemistry, Brno University of Technology. Within this team, we have more than 20 years of experience in this field, evidenced by almost 200 publications cited more than 1000 times.

FCH BUT is a proud holder of the HR Excellence in Research Award by the European Commission (<https://www.vut.cz/en/but/hr-award>).

Topic: **The study of bioaccumulation of selected contaminants in plants using the Laser-Induced Breakdown Spectroscopy method**

Supervisor: doc. Ing. Pavel Pořízka, Ph.D.

**Study program: Physical Chemistry**

Currently there is a big expansion in the development of nanomaterials that find their use in industry. As they become mass spread the risk of leaking into the environment increases and therefore it is necessary to monitor their influence on various ecosystems. Laser-Induced Breakdown Spectroscopy (LIBS) is an optical emission method suitable for elemental mapping of large sample surfaces. The information about biodistribution and bioaccumulation of material in the organism is crucial for correct evaluation of its toxic effect. The LIBS method can detect contaminants in plants with sufficient resolution. The goal of this work is to determine bioaccumulation and translocation of selected nanomaterials in plants and study of plasma activated water application on this bioaccumulation.

Topic: **Fluorescence spectroscopy in the study of properties of associative colloidal systems**

Supervisor: [Mravec Filip, doc. Ing., Ph.D.](https://www.fch.vut.cz/lide/mravec-filip-14999)

**Study program: Physical Chemistry**

This work is focused on the use of stationary, time resolved and microscopic fluorescence techniques in research of physical properties of associative colloids. The information obtained will be correlated with technological parameters of associative colloids such as solubilization and solubilization capacity, stability, size distribution, etc. The study will acquire not only skills in various techniques of fluorescence spectroscopy, but also in comparative techniques such as light scattering techniques.

Topic: **Utilization of prokaryotes for biotechnological production of polyhydroxyalkanoates and other high-value metabolites**

Supervisor: [Obruča Stanislav, doc. Ing., Ph.D.](https://www.fch.vut.cz/lide/obruca-stanislav-49647)

**Study program: Food Chemistry**

Thermophilic prokaryotes reveal numerous unique features which make them extremely interesting for microbial biotechnology. This dissertation work will be focused on the in-depth study of two very interesting thermophilic bacteria – gram-negative bacterium Schlegelella thermodepolymerans and also gram-positive bacterium Aneurinibacillus sp. H1. Both bacterial strains were recently described as very promising producers of polyhydroxyalkanoates – microbial polymers with the potential to replace petrochemical polymers in numerous applications. In this work, production polyhydroxyalkanoates will be studied employing numerous cultivation as well as molecular-biology approaches. Furthermore, tools of metabolic engineering will be used to improve the production of polyhydroxyalkanoates and other high-value metabolites.

Topic: **Biophysical characterization of polyhydroxyalkanoates in-vivo and ex-vivo**

Supervisor: [Obruča Stanislav, doc. Ing., Ph.D.](https://www.fch.vut.cz/lide/obruca-stanislav-49647)

**Study program: Biophysical Chemistry**

The focus of this thesis is the analysis of physicochemical properties of bacterial polyesters polyhydroxyalkanoates (PHA) with respect to their native form in bacterial cells (in-vivo) as well as concerning the characterization of the materials after extraction from the bacterial cell (ex-vivo). The goal is to understand the unique properties of these materials in the context of their biological functions and design and test employment of the materials in advanced applications (delivery systems, medical applications etc.).

Topic: **Fluorescence spectroscopy in the study of properties of associative colloidal systems**

Supervisor: [Mravec Filip, doc. Ing., Ph.D.](https://www.fch.vut.cz/lide/mravec-filip-14999)

**Study program: Biophysical Chemistry**

This work is focused on the use of stationary, time resolved and microscopic fluorescence techniques in research of physical properties of associative colloids. The information obtained will be correlated with technological parameters of associative colloids such as solubilization and solubilization capacity, stability, size distribution, etc. The study will acquire not only skills in various techniques of fluorescence spectroscopy, but also in comparative techniques such as light scattering techniques.

Topic: **Analysis of DNA binding proteins with a focus on their interaction with local DNA structures**

Supervisor: [doc. Mgr. Václav Brázda, Ph.D.](https://www.fch.vut.cz/lide/vaclav-brazda-198713)

**Study program: Biophysical Chemistry**

Local DNA structures play an important role in basic cellular processes such as replication and transcription. Recently, the presence of G-quadruplexes in DNA has been shown to be important for regulation in the cell, but also in the regulation of the life cycle of various viruses (HIV, HSV, EBV). These local structures are recognized by a variety of proteins. In this dissertation thesis, protein interactions with local DNA structures will be studied with a focus to cruciforms and quadruplex DNA. Physical, biochemical and molecular biological methods including the isogenic yeast system will be used to study the recognition of target structural motifs in the gene promoter region. Microscopic methods including confocal microscopy will also be used to study localization and interactions in cellular systems.

Topic: **Controlled release from hydrogels**

Supervisor: [Pekař Miloslav, prof. Ing., CSc.](https://www.fch.vut.cz/lide/pekar-miloslav-2035)

**Study program: Biophysical Chemistry**

Hydrogels still represent an attractive material in the formulating systems for the controlled release of biologically active substances. These are applied not only in medicine or food engineering but also, for example, in agriculture. Despite of the huge number of experimental works and of the knowledge of theoretical background of the release, the design and development of controlled delivery systems is still more matter of trial and error than of rational design rules. Even the very controlled release in real applications is not covered by clear procedures.

The thesis will thus focus on the generalization of published knowledge on the controlled release from hydrogel matrices, supported by student’s experimental work and modelling the release in particular with regard to in vivo conditions. Following the initial literature search partial tasks will be formulated including (all or selected) issues like:

• laboratory test studies of the release, influence of their parameters on the results, rational standardization of experimental protocols,

• diffusivity of the selected (model) drug as a function of the hydrogel or gelator concentration,

• transport and interaction of the selected (model) drug in different hydrogel systems, relation to problems observed in real applications; influence of conditions found in real environments (e.g., pH, temperature),

• modelling of drug release profiles with experimentally determined parameters and with regard to release and transport in real matrices (tissues).

The thesis will result in suggestion of a set of rational rules to select a suitable hydrogel for the encapsulation and controlled release of a given molecule in a particular environment.

Topic: **A physico-chemical contribution to discussion on soil organic matter**

Supervisor: [Pekař Miloslav, prof. Ing., CSc.](https://www.fch.vut.cz/lide/pekar-miloslav-2035)

**Study program: Biophysical Chemistry**

Soil organic matter, in a narrower sense, humic substances, has been subject of research for several centuries. Nevertheless, questions on its formation or character still have not been resolved. The traditional polymer theory seems to be replaced in the last two decades by supramolecular views, lately claims on the non-existence of the humic substances have become rampant, looking at the soil organic matter as a complex mixture of products at various degrees of the decomposition of decaying original plant or animal matter. Further, it can contain also metabolic products of the soil microorganisms.

After additional but in-depth literature search, the PhD study will be focused on one of or both following partial goals. 1) Thermodynamics and kinetics of the soil metabolic reactions with special regard to the synthesis of polyketides and their potential incorporation into the principal structural unit of the soil organic matter. 2) Colloid structures in the soil solution or in the soil aqueous leachates, their size, stability, diffusion behavior, aggregate character, chemical composition. Just hydrocolloids and water-soluble molecules are accessible to plants and thus are among key factors enabling and controlling their development and growth. Results will be evaluated also from the point of view of the current discussion on the origin, character, and stability of soil organic matter.

Topic: **Modelling of transport phenomena in biological environment**

Supervisor: [Pekař Miloslav, prof. Ing., CSc.](https://www.fch.vut.cz/lide/pekar-miloslav-2035)

**Study program: Biophysical Chemistry**

The development of various drug delivery systems is an area of active research. This research is focused mainly on chemical, biochemical, or physiological aspects. The movement of a delivery system in human body, to the point of the drug action is much less investigated. The drug transport to the targeted site where the drug’s chemical action should take place is essential for its proper function. This study will be therefore aimed at mathematical modeling of this transport based either on published data or data collected at the supervisor’s laboratory.

The work will be focused on the modeling of the diffusion of nano- and microparticles in model biological medium, especially in hydrogel or similar model of the extracellular matrix, or through biological membrane. These tasks will be solved using COMSOL packet. The tasks include also the construction of realistic structural model of the environment and the modelling support of the microrheological experiments in hydrogels performed in the laboratory where this PhD study will be realized. The aim of this study is obtaining a feedback for the design of the drug delivery systems.

Topic: **Development of techniques for fast assessment of soil quality and properties**

Supervisor: [doc. Ing. Jozef Krajčovič, Ph.D.](https://www.fch.vut.cz/en/people/jozef-krajcovic-73601)

**Study program: Chemistry, Technology and Properties of Materials**

Thermogravimetry appeared as a promising technique for fast assessing soil properties and showed a potential to replace current methods. These techniques are often costly and require a long experimental time, while thermogravimetry experiments require several hours. This work aims to search for new relationships between thermo-oxidative stability of soil determined using thermogravimetry and soil chemical properties (pH, content of biogenic elements including P, S and different forms of N, metals including Al and Fe), physical properties (texture and volume density) and biological indicators (microbial biomass, potentially mineralizable N, glomalin, and phospholipids contents and microbial emissions of carbon dioxide and nitrous oxide). These properties are known as indicators of soil quality. Therefore, the found correlations will be used to develop a complex soil quality index and models for predicting soil organic carbon stability.