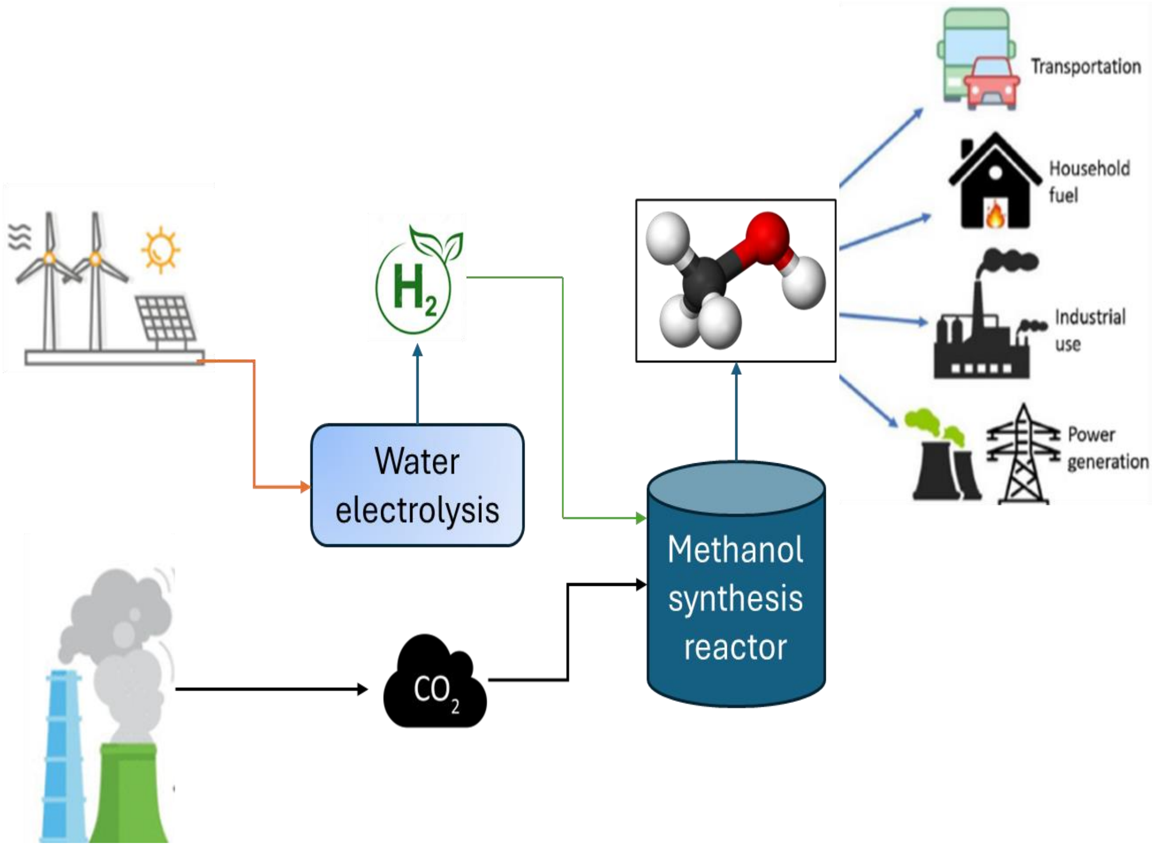
Doctoral Degree Study – List of Topics Offered in the Academic Year 2026 / 2027

Power to methanol process intensification



Renewable green methanol can play a crucial role in replacing fossil fuels and fossil-based raw materials with sustainable green alternatives. Renewable Power-to-Methanol (PtM) represents a promising technology for producing green methanol using captured CO_2 and green hydrogen generated from renewable energy sources. Various technologies for water electrolysis (for hydrogen production), carbon capture, and CO_2-based methanol synthesis are currently under development. However, process efficiency and high investment and operational costs remain major bottlenecks for these technologies. Process integration and intensification can significantly improve overall process efficiency and reduce costs. This project aims to design and evaluate various scenarios for the intensification of methanol synthesis, water electrolysis, and carbon capture processes, as well as their mutual integration, to enhance total efficiency and lower overall costs.

Advanced modelling skills using MATLAB and Aspen Plus, as well as experimental work skills, are required.

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Influence of thermal pretreatment on the leaching of Co and Li in Li-ion battery recycling

Advanced experimental work skills, as well as modelling skills, are required.

Recycling of Li-ion batteries has become one of the key challenges in global electrification and decarbonization strategies. To prevent the generation of hazardous waste and the loss of valuable metals such as cobalt (Co) and lithium (Li), safe and efficient recycling of Li-ion batteries must be an integral part of emerging battery-based, decarbonized technologies.

Various pyrometallurgical, hydrometallurgical, and direct recycling methods are currently under development. The efficiency of valuable metal leaching, as well as the environmental impact and cost of these processes, depends on several factors, including the choice of leaching agents, process conditions, and pretreatment of raw materials.

This project aims to investigate the influence of thermal pretreatment of material fractions from Li-ion batteries used in the leaching process on leaching efficiency, environmental impact, and overall process economics.

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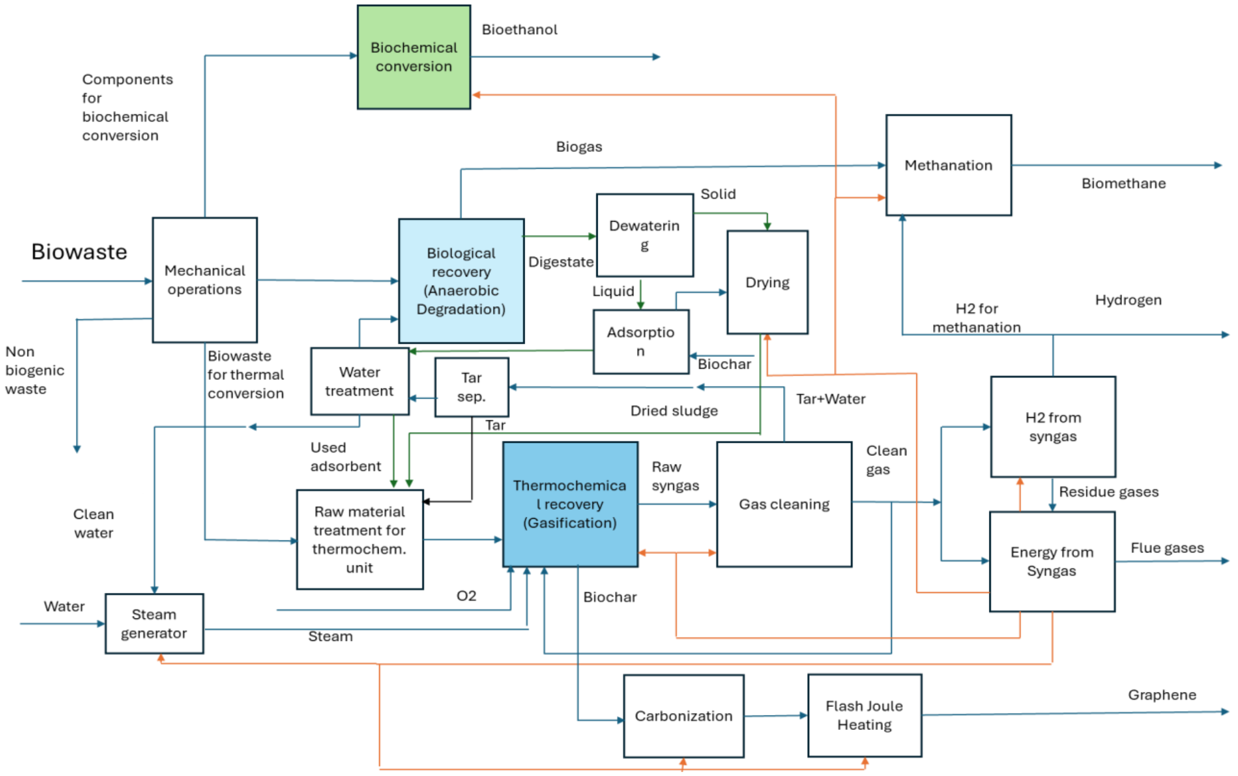
Upgrading biowaste thermal conversion products in an integrated biowaste biorefinery



The research project includes both experimental and computational components. The experimental work will provide data for model development and validation, while the computational work will involve building a computer model of the integrated process system capable of simulating and optimizing the system at an industrial scale...

The integration of various biological and thermal processes with a high degree of material and energy synergy within a biowaste biorefinery enables the complete conversion of biowaste and the upgrading of primary products into high-value raw materials and renewable energy. However, such mutual integration of biological and thermal processes, as well as the upgrading of their products, has so far been only minimally explored.

The goal of this project is to study and design processes for upgrading the primary products—biochar, bio-oil, and biogas—obtained from the thermal conversion of biowaste within an integrated biowaste biorefinery. The proposed upgrading processes will be connected with other units in the biorefinery, with a focus on minimizing waste generation and maximizing overall process efficiency.

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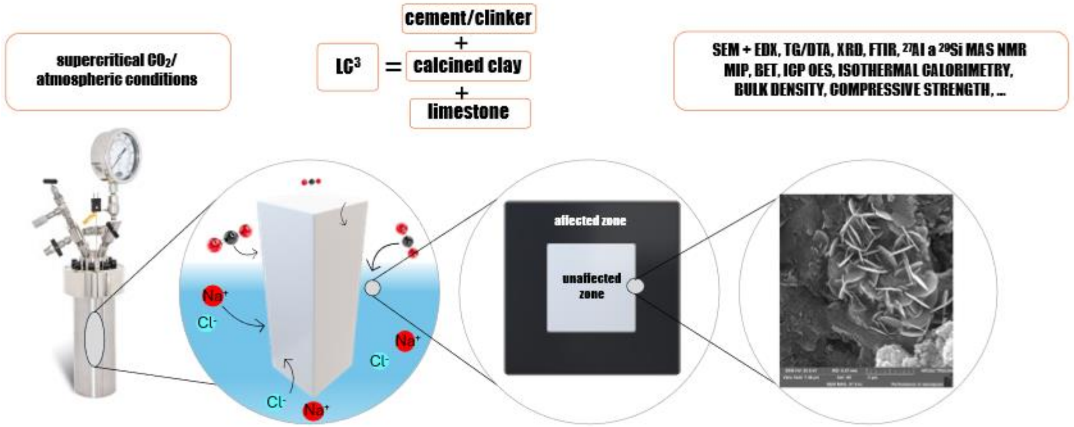
Resistance of LC^3 systems to the simultaneous effects of CO_2 and NaCl in various application environments



Limestone Calcined Clay Cement (LC^3) represents a new class of cementitious materials that has been the subject of intensive research primarily over the past two decades. Owing to the abundance of its raw materials and its significant environmental advantages, LC^3 has gained global attention as a promising alternative to conventional cement systems. However, in practical applications, LC^3 materials are often exposed to complex environments where simultaneous carbonation and chloride ingress occur, both of which can adversely affect their durability.

Despite growing interest, comprehensive and long-term studies on the durability of LC^3 systems under such combined exposures remain limited in the scientific literature. Furthermore, there is a notable absence of research addressing the performance of LC^3 materials in geothermal well environments, particularly in NaCl-rich geothermal water, which represents the most common type.

The primary objective of this project is to evaluate the long-term resistance of LC^3 systems under conditions simulating combined carbonation and chloride attack. Experimental investigations will be conducted under both atmospheric conditions and environments containing supercritical CO_2.

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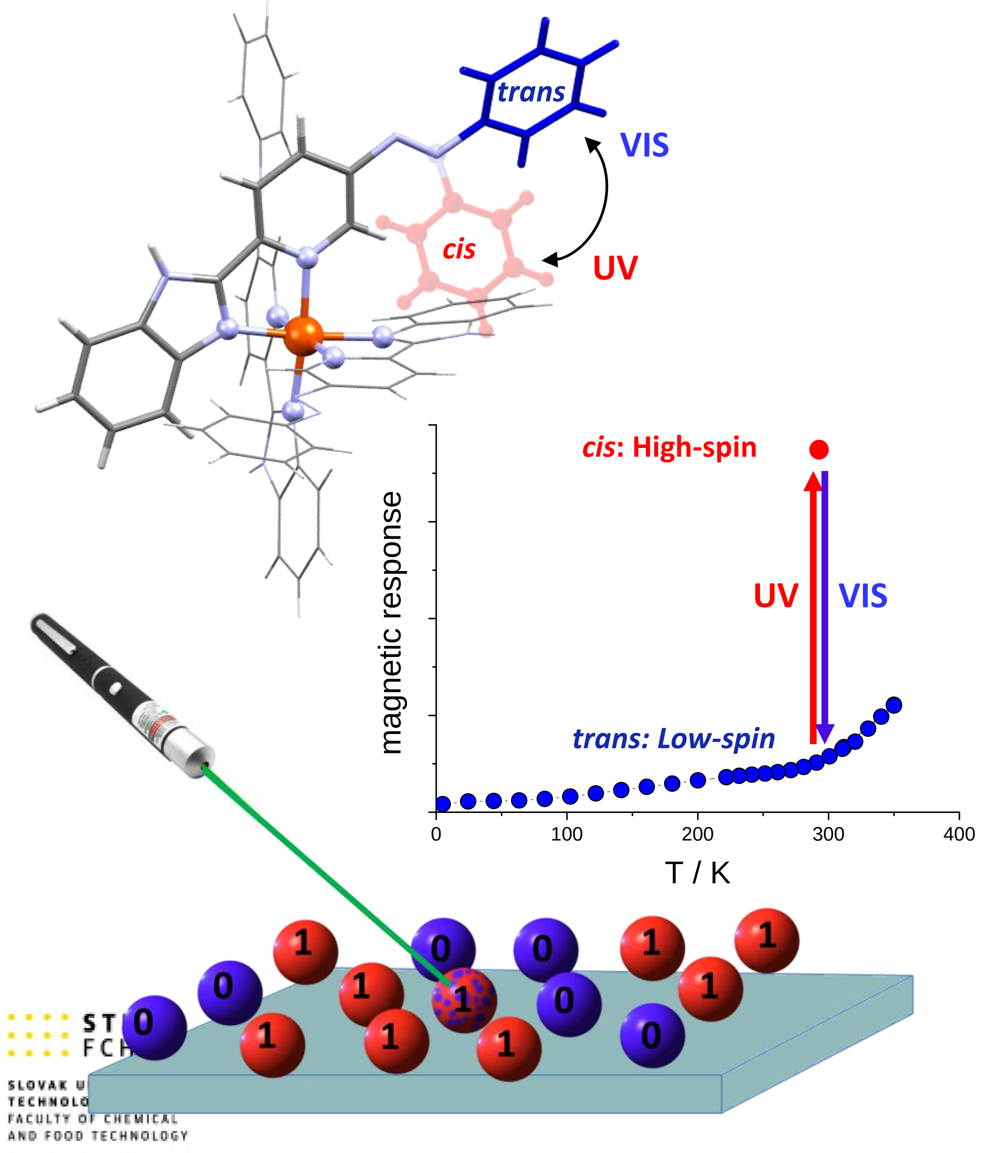
PhD Project: *Light-Controlled Spin Crossover in Iron Complexes: Toward Phototunable Molecular Materials;* **Supervisor:** *Prof. Ivan Šalitroš, DSc.* ivan.salitros@stuba.sk

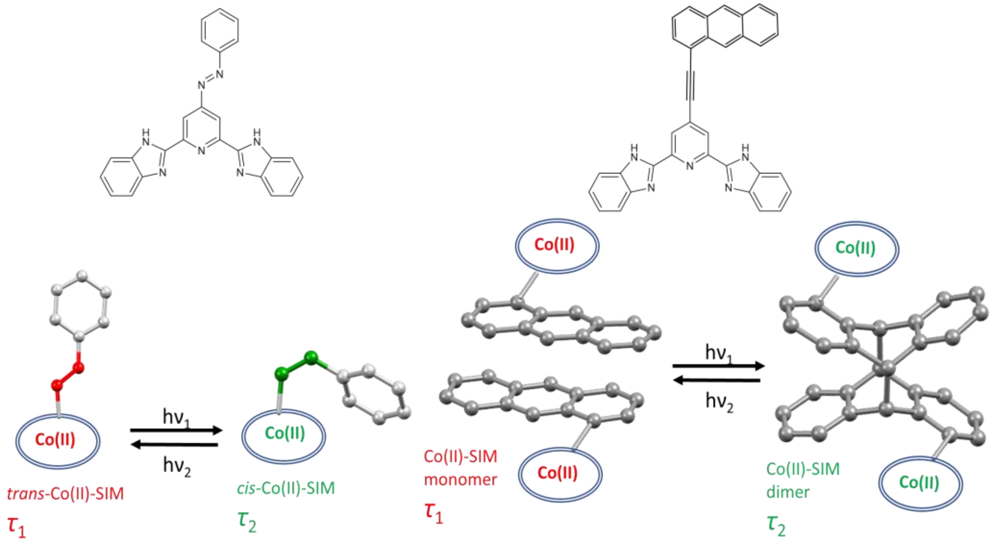


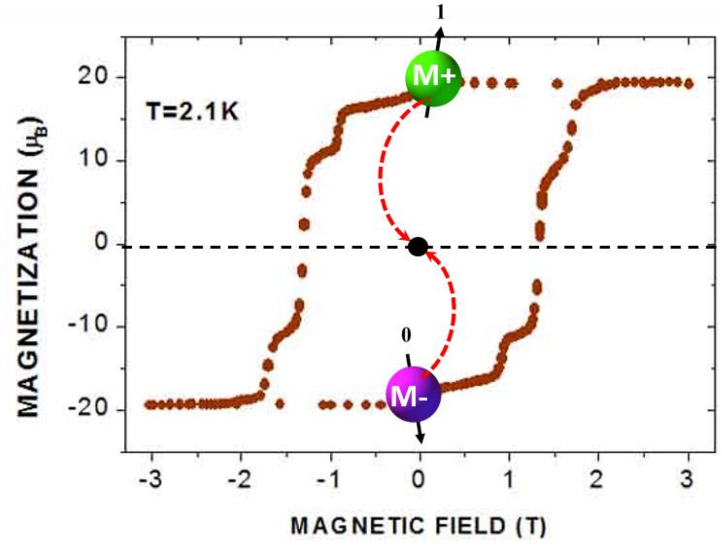
The PhD project will focus on the **synthesis and characterization of iron spin-crossover (SCO) complexes**, with particular emphasis on their **magnetic and photomagnetic properties**. The primary scientific goal is to **design, synthesize, and characterize new phototunable SCO materials** suitable for **surface deposition** using **sublimation** or **wet lithography techniques**.

A key aspect of the research involves the **incorporation of photoactive substituents**, such as **anthracene, azophenyl, and stilbene groups**, into **N-donor heterocyclic ligands**. This approach aims to achieve **light-controlled spin-state switching**, allowing external optical stimuli to modulate the magnetic behavior of the resulting iron complexes.

By integrating **synthetic chemistry**, **photochemical control**, and **magnetic characterization**, this project aims to advance the design of **smart molecular materials with tunable magnetic functionalities**. Such **phototunable SCO systems** hold significant potential for **nanotechnological applications**, including **high-density data storage**, **display technologies**, **MRI**, and **molecular spintronics**, due to their intrinsic **bi- or multistable magnetic behavior** at the molecular level.

PhD Project: *Smart Molecular Magnets: Slow Spin Dynamics in Photoresponsive Metal Complexes;* **Supervisor:** *Prof. Ivan Šalitroš, DSc.* ivan.salitros@stuba.sk





Proposed PhD project is focused on the **synthesis and comprehensive characterization of novel transition metals and/or lanthanide complexes**, with an emphasis on their **magnetism**. The primary goal is to develop materials that exhibit **slow relaxation of magnetization**—a key phenomenon underlying **single-molecule magnetism (SMM)**. Such systems are of great interest for **nanotechnological applications**, including **high-density data storage, display technologies** and **molecular spintronics**, due to their inherent **bi- or multistable magnetic behavior** at the molecular level.

The research will involve the **advanced organic synthesis of photoactive polydentate ligands**, particularly **N- and N,O-donor aromatic heterocyclic derivatives** bearing **photoresponsive substituents** such as **phenylazo** and **anthracene** groups. These ligands will serve as versatile building blocks for the preparation of **transition metal and lanthanide complexes**, primarily those of **Co(II)** and **Ln(III)** ions, where **slow magnetic relaxation phenomena** are expected to occur.

By integrating **synthetic chemistry**, **structural analysis**, and **magnetic studies**, this research aims to contribute to the development of **new single-molecule magnets** and to deepen the understanding of **magneto-structural relationships** in photoresponsive coordination systems.

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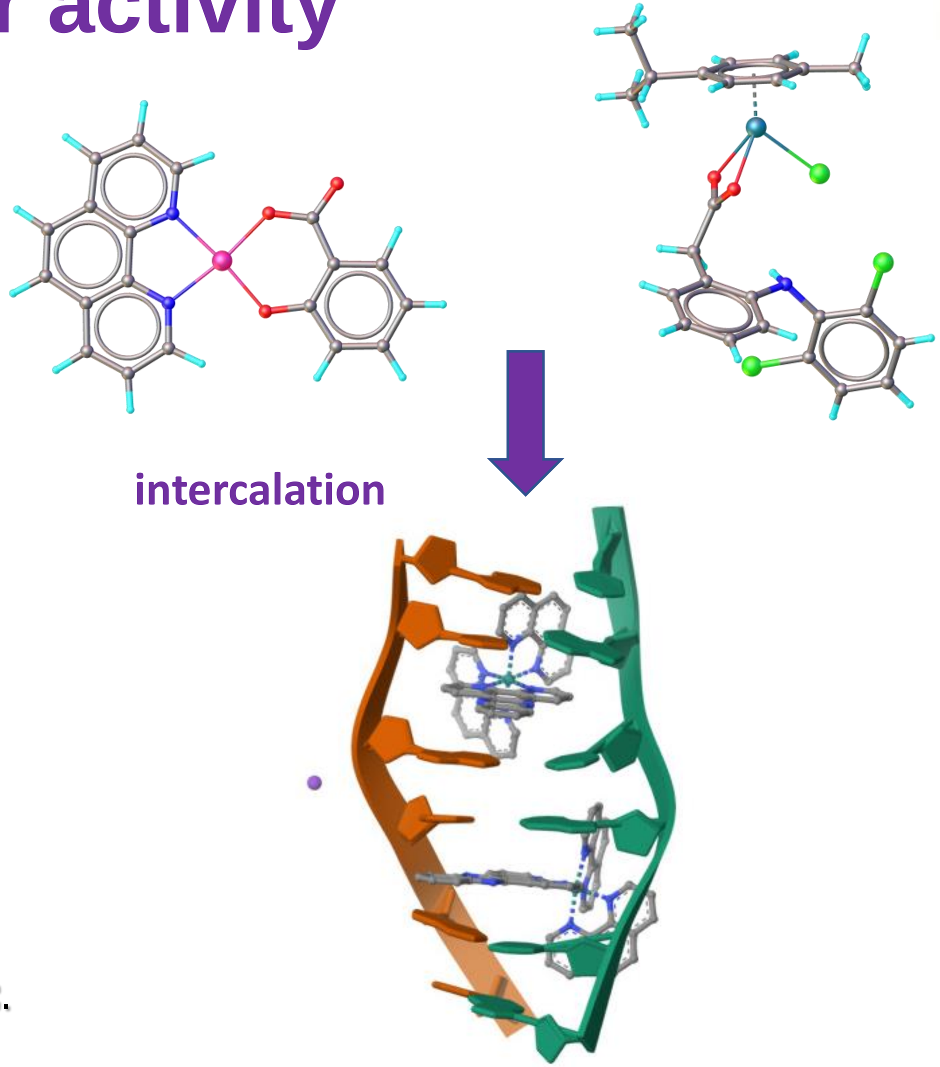
Development, synthesis, and structural study of ruthenium and palladium complexes with potential antitumor activity

Coordination chemistry offers a fascinating space where precise synthesis, detailed structural analysis, and the first steps toward biomedical applications meet. Ruthenium and palladium complexes form a stable but flexible platform that allows us to design structurally novel molecules and investigate their chemical behavior and potential biological activity.

The dissertation focuses on the synthesis of new ruthenium and palladium complexes and their study. The prepared compounds will be characterized by spectral methods and X-ray structural analysis. Selected compounds will be studied for their interaction with DNA and albumin, as well as their anticancer activity.



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Quantum crystallography of transition metal complexes: precise structure, electron density, and intermolecular interactions

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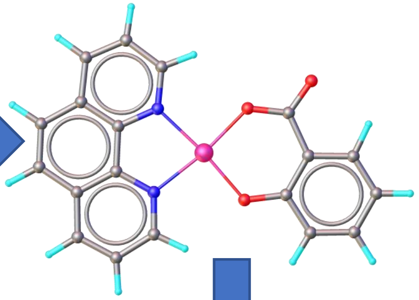

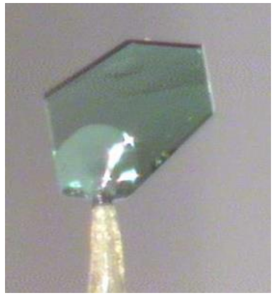

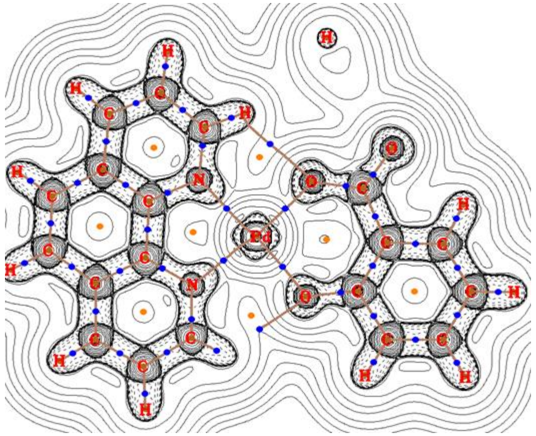

Transition metal complexes are among the most interesting chemical systems in terms of coordination, reactivity, and electron structure. Their rich chemical variability, the presence of heavy atoms, complex bond topology, and extensive spectrum of intermolecular interactions pose a challenge to traditional crystallographic approaches.

Modern quantum crystallography overcomes these limitations by combining high-precision single-crystal X-ray diffraction with computational methods that allow direct investigation of the experimental electron density and its topological characteristics.

The dissertation focuses on the synthesis and crystallographic analysis of transition metal complexes. The prepared compounds will be characterized X-ray structural analysis. Structural analysis will be performed using methods of quantum crystallography (multipole refinement, Hirshfeld atom refinement, Hirshfeld surface analysis, and topological analysis).

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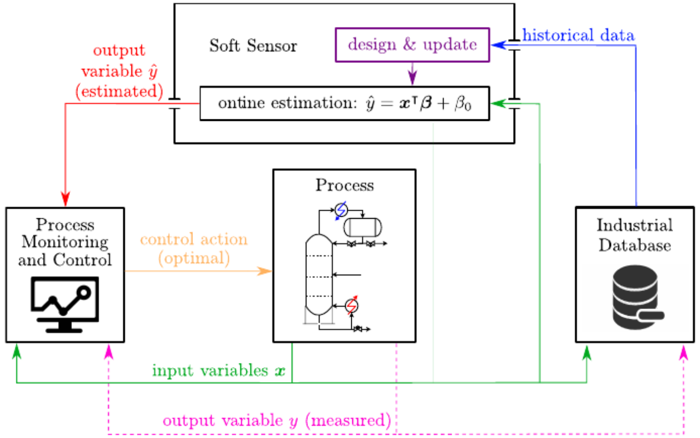
Development of Reliable and Explainable Models for Industrial Monitoring, Optimization, and Control



Safe and sustainable process systems, which constitute the backbone of a modern, developed society, require sensing of key process variables, estimation of unmeasured variables, and application of actions that steer the systems towards desired goals. Automation of human decisions in such tasks would make these decisions become fast, reliable, and error-free. A key technology on the rise in this context is the use of combined mathematical modelling and statistical learning to gather information through software (soft) sensors to monitor, assess, and steer the behaviour of dynamic systems (e.g., industrial processing plants, water, gas and energy networks, or manmade machines and vehicles) into desired operating regimes.

The delivered tools will exploit domain knowledge – making the designed mathematical models explainable – and assess and improve the information content of the data – making the models reliable and fit for industrial needs.

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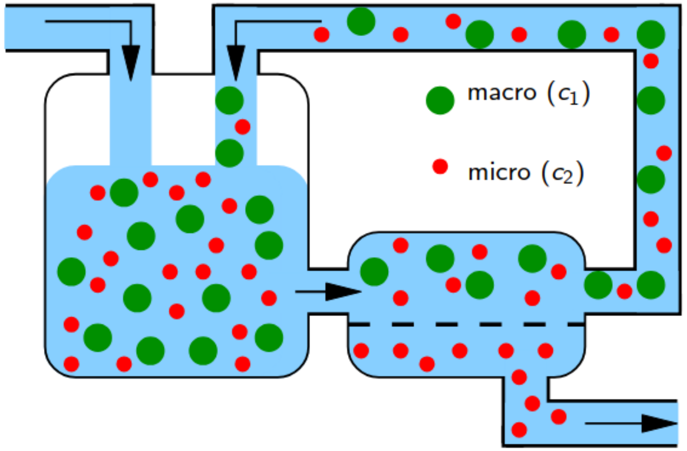
Modelling, Optimal Design and Optimal Operation of Membrane Processes



Membrane processes are crucial in various industrial sectors due to their efficiency. The proposed research aims to develop a framework combining advanced mathematical modeling with optimization algorithms to achieve optimal design and operation of membrane processes.

The study will involve the development of mathematical models that capture the complex phenomena involved in membrane processes, considering factors such as mass transfer, fluid dynamics, and membrane fouling. Furthermore, the research will focus on optimizing the design parameters of membrane systems to enhance performance, minimize energy consumption, and reduce environmental impact. Finally, the proposed framework will facilitate real-time optimization strategies for the optimal operation of membrane processes, ensuring efficient and sustainable operation under varying operating conditions.

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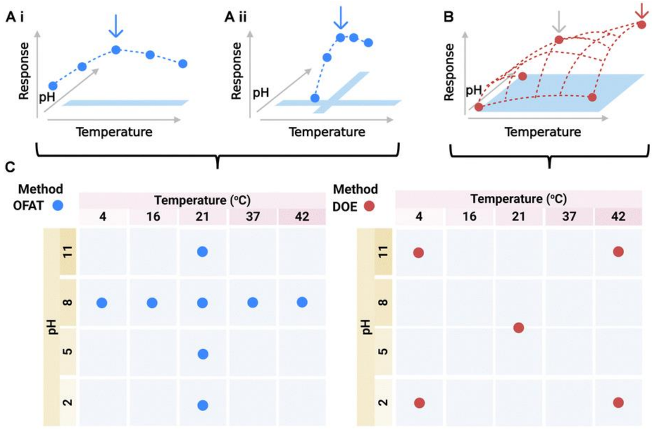
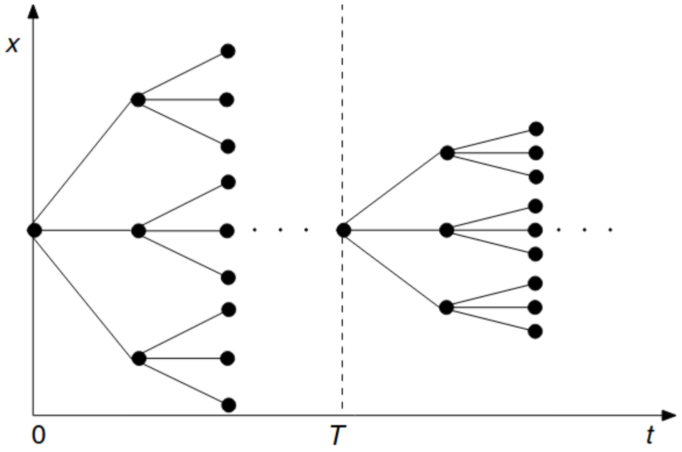
Robust Design of Optimal Experiments





This project develops approaches to robust model-based design of experiments in the context of maximum-likelihood estimation. The developed approaches provide robustification of model-based methodologies for the design of optimal experiments by accounting for the effect of the parametric uncertainty.

The problem of robust optimal design of experiments in the framework of nonlinear least-squares parameter estimation is well known, yet the presently existing methods do not solve it to a full extent. A promising step towards solving the problem appears to be based on multi-stage robust optimization. The multi-stage formalism can aid in identifying experiments that are better conducted in the early phase of experimentation, where parameter knowledge is poor.

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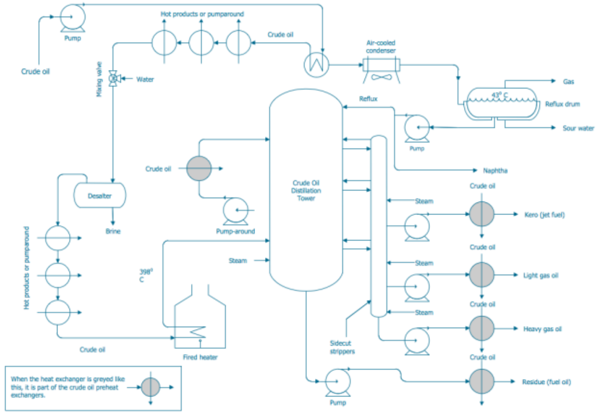
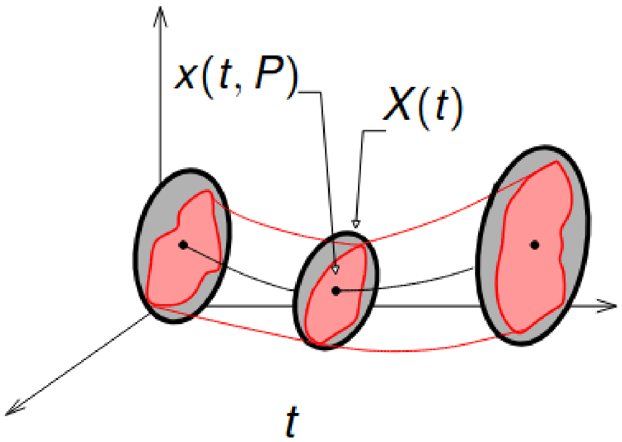
Set-based Control of Nonlinear Systems





As the computers and algorithms get faster, many new control concepts become tractable and can be developed. Set-based control is one of these, where the primary use of sets is in enveloping a space of possible evolutions of variables of a system over time. If these envelopes can be obtained in reasonable time, many properties of dynamic systems such as stability or robustness can be reasoned about.

The first goal of the thesis is to build a novel type of multi-base set arithmetics that combines elements such as interval analysis, convex-set theory, and polynomial functions to achieve the best trade-off between accuracy of representation and the burden associated with the underlying calculations to obtain the envelopes. The second goal of the thesis is to develop methods of synthesis of controllers that can be used for safe and reliable control of nonlinear systems. The project of the thesis will be finished with a successful demonstration of the developed techniques on a laboratory plant.

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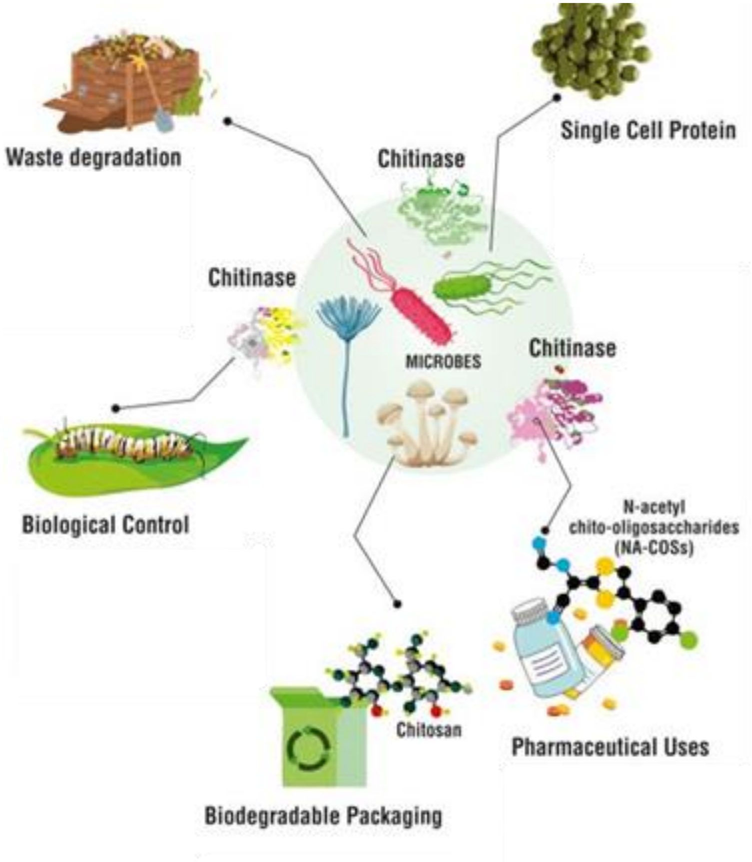
Engineering of Enzymes for Sustainable Bioprocesses



Srivastava, A. & Srivastava, S.: Chitinase enzyme: sources and application, In: Bioactive Microbial Metabolites, Academic Press, 2024: pp. 151–164

PhD Position in Biotechnology (Laboratory of Applied Biocatalysis)

We are seeking a motivated PhD candidate to join a project focused on discovering and engineering chitin-active enzymes. The work combines metagenomic screening, protein expression, and enzyme redesign.

Main responsibilities

Identification of new enzymes from metagenomic datasets

Expression, and purification of selected candidates

Biochemical characterization and redesign of enzyme variants

Data analysis and preparation of publications

Requirements

Master’s degree in Biotechnology, Biochemistry, or a related field

Background in molecular biology or protein biochemistry is an advantage

Strong interest in metagenomics and enzyme engineering

Good communication skills in English

We offer

Full time PhD position in a dynamic research environment

Access to modern laboratory facilities

Training and support in advanced experimental and computational methods

Supervisor: Assoc. Prof. Martin Rebroš, PhD.
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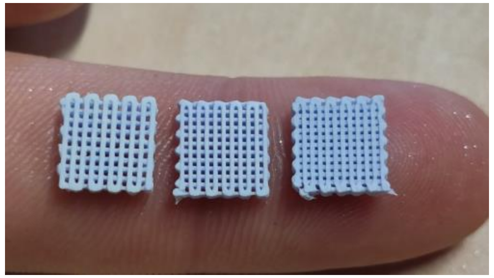
Multimaterial based bioceramics with tunned biological response.



The family of additively manufacturable hydroxyapatite (HA) personalized alveolar augments, will be in a focus of the development. The exploration of a material-modification strategy based on high temperature HA reactions, using therapeutic ion doping with a tuned release will be investigated. In vitro inflammatory and angiogenesis protein response will be probed in cooperation with research partners, including osteogenesis behavior of material investigated with balanced remodeling are considered as route to reach the balanced bioactivity during bone healing as the main objective.

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Mullite based ceramics produced with additive manufacturing.

In situ components reaction will be used for preparation of mullite ceramic after its shaping using fused filament 3D printing of ceramics. The effect of chemical composition of mullite forming components, their ratios and morphology of the particles will be used to investigate their effect on the final properties of prepared ceramic printouts. The investigation will also include the effect of printout treatment during debinding and sintering on resulting microstructure, phase composition and mechanical strength of prepared model 3D structures.

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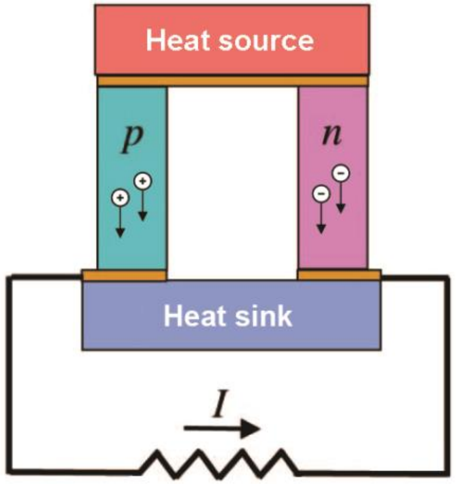
Thermoelectric structures produced with multimaterials FDM additive manufacturing.



Fused deposition modeling (FDM) of ceramics will be used for printability investigation of the specific shape designs selected as host structures for other material components inclusions. The 3D printed host structures will be designed to adopt thermoelectric material components $\boldsymbol{p}$ and $\boldsymbol{n}$, to verify the additive manufacturing process and using multimaterials printing such as ceramics or metals. The main objective is to verify proof of concept in FDM of thermoelectric structures. The functionality of the structure and selected ceramic will be verified for its suitability to act as heat acceptor and heat sink.

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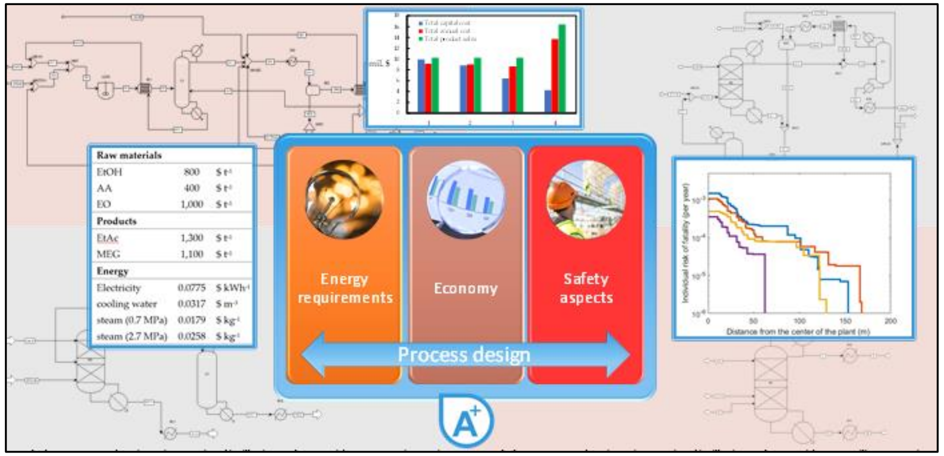
Enhancing Chemical Process Safety Through a Dynamic Digital System for Industry 4.0

The general objective of the project is to develop a software framework – a digital twin – as a dynamic digital system for hazard identification in complex chemical processes. The framework will follow to the principles of the HAZOP technique, as it has the potential to control the mechanisms of both steady-state and dynamic simulations of the targeted process. Understanding the nonlinear behavior of the process and the evolution of operating parameters during failure modes enables effective improvements in safety barriers during HAZOP analysis. The objectives of this research are as follows:



- To develop a digital twin of a chemical process of the real industrial unit;
- To present methods for evaluating nonlinearity indicators in chemical processes for hazard identification;
- To present a compact framework methodology of model-based HAZOP for a digital twin.

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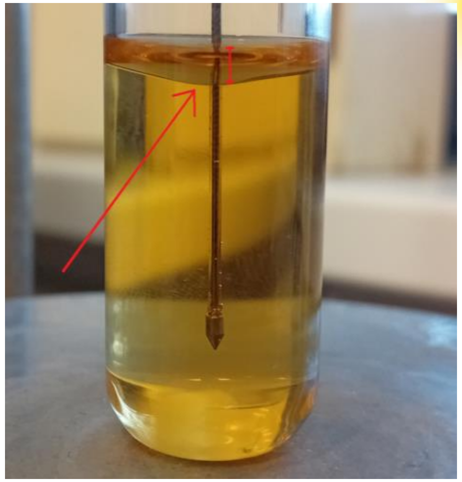
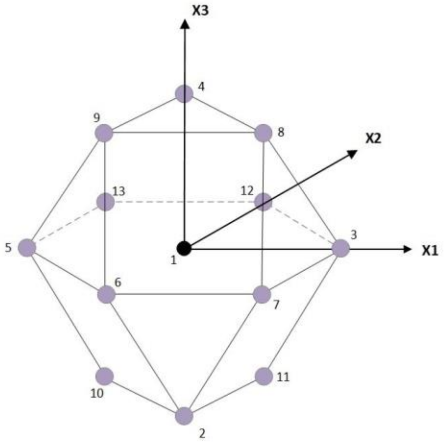
Enhancing Novel Microextraction Techniques Through Experimental Design

The proposed project aims to enhance microextraction techniques for analysing food commodities by integrating experimental design principles into the development of novel solid-phase microextraction (SPME) methods, specifically **SPME Arrow** and **thin-film SPME**. These techniques offer faster extraction, greater sorption capacity, and improved reproducibility compared to traditional configurations. Moreover, due to their high surface-to-volume ratio and porosity, the project will highlight testing nanofibers as sorbent materials for these extraction techniques. The objectives of this research are as follows:





The objectives of this research are as follows:

- Incorporating the design-of-experiments approach for the development of microextraction techniques
- Testing of the proposed microextraction techniques
  with commercially available sorbents for analysis of novel food commodities and meat-based products
- Exploration of various polymeric nanofibers and nanofiber composites as alternatives to traditional sorbents.

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