Programme title: Chemistry, Technology and Properties of Materials

Mode of study: full-time

Topic title: Alternative inorganic binders based on accelerated carbonation curing

Supervisor: Ing. Eva Bartoníčková, Ph.D.

Specialist supervisor: Ing. Jiří Másilko, Ph.D.

Description: This dissertation focuses on the study of accelerated carbonation curing of synthetic phases within the $CaO–SiO_2$ system, specifically wollastonite, larnite, calcium olivine, rankinite, and hatrurite. The effects of external processing conditions on the kinetics and mechanisms of carbonation in laboratory-prepared pure phases are investigated, and the resulting mechanical properties as well as the characteristics of the formed carbonation products are evaluated. The acquired knowledge is subsequently applied to selected secondary raw materials originating from industrial production and various recycling processes. Particular attention is paid to the effect of foreign ions present in secondary raw materials on the carbonation process and on the formation and stability of carbonation products.

Topic title: Functionally modified C–S–H gels as a binding phase in 3D printing technology

Supervisor: Ing. Eva Bartoníčková, Ph.D.

Specialist supervisor: doc. Ing. František Šoukal, Ph.D.

Description: This doctoral dissertation focuses on the study of functionally modified C–S–H gels as a binding phase in the 3D printing of silicate materials, with particular emphasis on the Direct Ink Writing method. The research is focused on synthesizing C–S–H gels with deliberately tailored chemical compositions and functional properties that influence their hydration behavior, rheological characteristics, and material response during the 3D printing process. Attention is devoted to the effect of functional modification on the development of the binder microstructure and its interaction with the extrusion and shear conditions characteristic of the Direct Ink Writing technique. The dissertation further includes a systematic investigation of the relationships between printing process parameters, hydration kinetics, and the controlled distribution of modified C–S–H gels within the printed structure. This dissertation aims to contribute to a deeper understanding of the relationships between the chemical nature of the binding phase and its applicability in additive manufacturing technologies for producing silicate materials.

Topic title: Titanium-Based Semiconducting Heterojunctions Derived from Polymeric Precursors for Photocatalytic Degradation of Pollutants

Supervisor: Ing. Eva Bartoníčková, Ph.D.

Specialist supervisor: Ing. Vojtěch Jašek, Ph.D.

Description: The dissertation focuses on the preparation of titanium-based semiconducting heterojunctions and their application in photocatalytic processes. The selected approach for ceramic material synthesis based on polymer-derived precursors enables targeted control of chemical composition, phase composition, and microstructure of the resulting materials, which is crucial for

optimizing their functional properties. The photocatalytic performance will be evaluated using selected model organic pollutants with the aim of elucidating the relationships between structure, properties, and functional parameters of the materials.

Topic title: Synthesis and Characterization of Bio-based Reactive Systems for Selected Material Applications

Supervisor: Ing. Silvestr Figalla, Ph.D.

Specialist supervisor: Ing. Vojtěch Jašek, Ph.D.

Description: The motivation for this doctoral thesis arises from the urgent need to transform the chemical and materials industries toward the principles of sustainable development, aiming to reduce the dependence on fossil resources that currently dominate the production of synthetic polymers. The primary driving force is the increasing legislative and social pressure to utilize renewable raw materials, which can serve as more environmentally friendly alternatives to conventional petrochemical monomers without compromising the performance properties of the resulting materials. A key aspect of this research is, therefore, the design and synthesis of novel reactive resins that partially or fully utilize renewable resources as building blocks for macromolecular substances. Particular attention is paid to the functionalization of natural precursors with reactive groups, such as acrylates and methacrylates, enabling their subsequent processing via modern technologies, including additive manufacturing or the preparation of coatings and adhesives. A significant scientific challenge is represented by the utilization of itaconic acid, which, as a biotechnologically accessible unsaturated dicarboxylic acid, offers a unique platform for the synthesis of fully renewable resins capable of radical polymerization. However, the objective of this work extends beyond synthesis alone; it aims for a comprehensive understanding of the structure-property relationships between bio-precursors and their reactivity, which is essential for optimizing curing processes. A detailed study of physicochemical characteristics, along with the analysis of the mechanical properties of the prepared resins, aims to verify whether these novel materials can compete with established commercial products in targeted material applications—such as specialized resin systems, protective coatings, or 3D-printed prototypes—thereby contributing to the broader implementation of sustainable chemistry in practice.

Topic title: Development and Characterization of Photopolymer Materials for Advanced Photopolymerization Technologies

Supervisor: Ing. Silvestr Figalla, Ph.D.

Specialist supervisor: Ing. Vojtěch Jašek, Ph.D.

Description: Photopolymerization technologies represent a vital tool for the preparation of micro- and macro-structured polymeric materials with precisely controlled geometries and properties. Methods based on controlled photopolymerization, including two-photon polymerization (2PP), enable the creation of structures with high spatial resolution and find applications across a wide spectrum of fields—ranging from micro-optics and functional surfaces to micro- and nanostructured systems and medical applications. The scope of this doctoral thesis involves research into molecular structure design, synthesis, and the modification of the resulting photopolymer materials, alongside the study of their behavior during controlled photopolymerization. The work will focus on the relationships between the chemical structure of the resins, their reactivity, polymerization kinetics, and the resulting

physicochemical and functional properties of the cured structures. A key component of the research will be the investigation of how the composition of photopolymer systems (types of monomers and oligomers, functional groups, photoinitiators, and potential additives) influences the photopolymerization process and the quality of the fabricated structures across various scales. The objective of the thesis is to contribute to the advancement of knowledge in the field of high-performance photopolymer materials and their application in advanced technologies based on controlled photopolymerization.

Topic title: One-Part Alkali-Activated Systems

Supervisor: doc. Ing. Lukáš Kalina, Ph.D.

Specialist supervisor: Ing. Vlastimil Bílek, Ph.D.

Description: In the research of alkali-activated binders, one-part systems are becoming increasingly popular, where the activator is pre-mixed with the precursor in a solid state, so when using this binder, it is only necessary to add water, similar to conventional Portland cement. From a practical point of view, in addition to the established preparation procedures, it is also advantageous that the storage of highly alkaline solutions and handling with them is eliminated. On the other hand, certain pitfalls are the hygroscopicity of the activator, its dissolution in water, the potentially different kinetics of the formation of reaction products compared to conventional liquid activators, and also the low efficiency in alkaline activation, since activators with a lower pH are usually used in the smallest possible doses due to economic and ecological aspects. One-part systems also differ from two-part systems in terms of rheology and function of admixtures. The work is therefore focused mainly on the early stages of alkaline activation of one-part systems (rheology, temperature development, reaction processes, functionality of organic admixtures) and optimization of their composition also with regard to long-term properties. The work will also include a study of the microstructure of these systems and identification of the forming hydration products.

Topic title: Non-fullerene acceptors based on high performance dyes and pigments for organic photovoltaics

Supervisor: prof. Ing. Jozef Krajčovič, Ph.D.

Specialist supervisor: Ing. Martin Cigánek, Ph.D.

Description: The work will focus on the targeted synthesis and advanced chemical modification of organic materials based on pigments and dyes, by synthesizing their polymers and co-polymers for applications in the fields of organic electronics. The design of molecules will be aimed at studying the effect of chemical derivatization on the electron-accepting, as well as optoelectric properties of the resulting materials, in relation to targeted applications, especially in the field of photonics.

Topic title: Organic-inorganic and all-inorganic trihalide perovskite materials for applications in neuromorphic electronics

Supervisor: Ing. Jan Pospíšil, Ph.D.

Specialist supervisor: Ing. Stevan Gavranovič, Ph.D.

Description: This work deals with the preparation and characterization of various types of perovskite materials, which are promising for use in the field of neuromorphic electronics, i.e. for the future development of neuromorphic systems, computers and advanced memory devices. Attention will be focused primarily on the characterization of the optical and electrical properties of materials, especially in the form of thin layers. The use of these materials in memristive devices and monitoring of their switching response will also be studied. The work will be carried out with the support of the GACR project and in cooperation with other institutions, including foreign ones (e.g. INM-CNR in Italy and INAM in Spain).

Topic title: Synthesis and Characterization of Novel Reactive Resins as a Sustainable Matrix Option for Composite Materials Manufacturing

Supervisor: doc. Mgr. Radek Přikryl, Ph.D.

Specialist supervisor: Ing. Silvestr Figalla, Ph.D.

Description: Global pressure to reduce the environmental burden and dependence on fossil fuels represents one of the greatest challenges in contemporary materials engineering. In the context of the current climate crisis, sustainable solutions are required for industrial applications.

Composite materials, which are essential for modern industry due to their exceptional combination of strength, low weight, and durability, often rely on resin matrices derived from non-renewable (fossil) sources, thus creating a significant environmental footprint. The main goal of current materials research is therefore the transformation of these systems, specifically through the development of new, ecologically friendly resins.

Innovation in this direction focuses on the synthesis of reactive precursors derived fully or partially from renewable resources, and on the valorization—the chemical transformation—of commercial materials or waste into valuable resin precursors. This approach represents an industrially attractive path toward a more sustainable future for composite materials.

This doctoral thesis will actively engage in solving this key issue, as its main ambition is to introduce a sustainable approach to the manufacturing of composite matrices. The work will target the design and synthesis of novel reactive resins, serving as the continuous phase of the prepared composite systems, and will include a detailed analysis of the chemical structure and functional properties of the prepared reactive precursors. An integral part of the research is also the study of the physicochemical properties of the synthesized products and the subsequent testing of the corresponding composite products in terms of their mechanical and thermomechanical properties. The conclusions of the thesis should summarize the results achieved with regard to practical application and provide a proposal for future work, thereby contributing to knowledge in the field of sustainable chemistry and materials engineering.

Topic title: The influence of methanogens and sulfate-reducing bacteria on the corrosion behavior of magnesium alloys in anaerobic environments

Supervisor: doc. Ing. Jaromír Wasserbauer, Ph.D.

Specialist supervisor: Ing. Leoš Doskočil, Ph.D.

Description: The corrosion behavior of magnesium materials has been studied for several decades in various environments, and a number of corrosion protection strategies have been developed. However, current research neglects the importance of microbially influenced corrosion, which can be crucial for magnesium material applications. This work will conduct a comprehensive study of the corrosion of magnesium alloys under anaerobic conditions with the aim of determining the influence of methanogenic archaea, sulfate-reducing bacteria, and their mixed cultures on the corrosion process. The results obtained will lead to the formulation of the first comprehensive concept of the corrosion mechanism of magnesium alloys in the presence of the microorganisms under investigation. Furthermore, the first functional inhibitor providing simultaneous protection against corrosion and microbial action will be proposed.

Topic title: Advanced materials for transparent solar cells

Supervisor: prof. Ing. Martin Weiter, Ph.D.

Specialist supervisor: Ing. Matouš Kratochvíl, Ph.D.

Description: Semitransparent organic solar cells (ST-OSCs) offer a disruptive opportunity to combine energy harvesting with protection against excessive thermal radiation, finding applications as photovoltaic windows or greenhouses. A key challenge lies in the inherent balancing of power conversion efficiency (PCE) and average visible transmittance, which current materials do not provide. To address this, novel semiconductors with strong FR-NIR absorption will be synthesized and the fundamental electronic processes on molecular level determining their optoelectronic properties systematically investigated.

The work will deal with the preparation and characterization of materials - organic semiconductors, which are perspective for use in the field of organic and hybrid photovoltaics. Organic solar cells will be prepared and characterized by methods of material printing and other methods and their properties will be studied. Attention will be focused on characterization of optical and electrical properties of materials and solar cells. The aim is to optimize the properties of solar cells with respect to their specific application possibilities. It is expected that the PhD student will be involved in an national research project focusing on organic photovoltaics.