Thesis topics of the Department of Physical Chemistry, 2022/23/1.

Attila Bényei:

Regulatory issues for polymorph or co-crystal modifications of Active Pharmaceutical Ingredients. Chemical engineer BSc/MSc, 1 person, free,
APIs often form different solid state structures either as polymorphs or via co-crystallization with other compounds. The task is the comparison of the regulatory issues in this field published by US (FDA), European (EMA) and other agencies. It is important to identify the differences and trends in this field as we as their engineering consequences in pharma industry.

Use of crystallographic database in comparison of solid state structures. Chemical engineer BSc/MSc, 2 persons, 1 free)
Comparison of solid state structures is very important in the comprehensive analysis of metal complexes or biologically active organic molecules. The Cambridge Structural Database contains over 1 Million published structures. The task is to identify similar structures of a given compound family from the CSD and analysing their conformation in the solid state, describe the secondary interactions in the lattice and find links to the physico-chemical properties.

Oldamur Hollóczki:

Mechanistic investigation of the reactions between imidazolium salts and carbon disulfide (chemistry BSc, 1 person, not free)

Noémi M. Nagy and Eszter Mária Kovács:

Structural changes of lanthanide bentonites by heat treatment (Chemisrty or Chemical engineer BSc, 1 free)

Levente Novák:

Formation of amide bond by thermal reaction in polar aprotic medium (MSc thesis, 1 person)
The amide bond formed by condensation between carboxyl and amino groups is of great importance for the synthesis of organic macromolecules owing to its hydrolytic stability and polar nature. In protic solvents (thus in water) it can only be formed indirectly from the appropriate amine and carboxylic acid due to the dissociation of these precursors. It is less known however, that in aprotic solvents amides can also form directly by thermal condensation.

The reaction is probably made possible by the changed acid-base conditions, while the reaction equilibrium is shifted to the direction of the formation by the water solvation capacity of the solvent. We plan to investigate the kinetics of the reaction with small molecules, as well as with polymers, with special emphasis given to the acid-base conditions existing in the aprotic solvent.

Synthesis and characterization of functionalized macromolecules (MSc thesis, 1 person, filled already)

The properties of macromolecules are strongly influenced besides their chemical composition by other factors, as e.g. the structure of the carbon chain, the molecular weight and weight distribution of the polymer, spatial position of certain functional groups and their mutual distance. Macromolecules functionalized by suitable groups can be excellent ligands for different metal ions and the complexes so formed possess several advantages over the complexes of small molecules (decreased diffusion rate, easy separability, specific selectivity, kinetic stability). The synthesis of these macromolecules with specific properties is performed partly by linking together monomeric units, partly by the modification of existing polymers (called platforms).

Purification of the product from the starting materials and the byproducts of the reaction is an important step. Following the synthesis and the purification we will investigate the main properties of the macromolecules formed and/or the behavior of their most suitable metal complexes for a given area of application (colloidal catalysis, environmental protection, magnetic contrast agents).

Gyula Tircsó and Balázs Váradi:

Synthesis and characterization of responsive MRI probes (Chemistry MSc, 2 persons, not free)

Magnetic resonance imaging (MRI) is a non invasive diagnostic tool that has long been used to obtain anatomical and functional images. In recent years, the new field of molecular imaging has emerged which looks for information at the molecular level by visualizing the concentration and function of bioactive molecules (glucose, citrate etc. concentration) or physiological parameters (pH, pO2, etc.). The project aims to develop new systems for the imaging pH by MRI relying on our recent results (using platforms obtained as a results of fine tuning of physicochemical parameters of the complex), as well as coordination chemical characterization of the resultant complexes (stability and inertness of the complexes, relaxation properties etc).