Thesis topics of the Department of Physical Chemistry, 2023/24/1.

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, 1 person, 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.

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).

Oldamur Hollóczki:

Modelling the interactions between nanoplastics and proteins (1 student, and the position is occupied.)
The student will investigate the effect of nanoplastics on proteins that play an important role in carcinogenesis and the formation of neurodegenerative diseases. The results will contribute to the understanding of the potential impact of micro- and nanoplastics, and the underlying mechanisms of action. The ideal candidate has a basic molecular modelling and computational chemistry background.

Rare Earths Research Group:

Complexes of the lanthanide ions (Ln3+) have been utilized in medical applications due to their widespread magnetic, photophysical, and nuclear properties. Owing to their toxicity the Ln3+ ions are must chelated using multidentate ligands. Beside the traditional pendant arms, the picolinate metal binding moiety is explored more extensively nowadays. The proposed project therefore aims at the development and synthesis of a monopicolinate based chelator derived form the 2,2'-oxybis(ethylamine) diamine possessing three acetate pendant arms (OBE3APA). The research will focus on the synthesis of the ligand and characterization (stability, formation and dissociation kinetics) of their complexes formed with metal ions of biomedical relevance (Bi^{3+}, Gd^{3+}, Sc^{3+} etc.).