The Institute of Catalysis and Surface Chemistry of the Polish Academy of Sciences conducts experimental and theoretical research in the broadly understood fields of surface chemistry, colloids, nanostructures of soft matter, materials chemistry, and enzymatic catalysis. Within the scope of activities in the Doctoral School of Quantitative and Natural Sciences, the research includes the application of advanced molecular modeling methods in the following areas:

I. Carbohydrate Conformation

Carbohydrates are a diverse group of natural biomolecules that play a key role in living organisms as a primary energy source, building materials, and regulators of various metabolic processes, affecting both human health and ecosystem functioning. Research on these molecular systems focuses on a detailed analysis of dynamic structure (conformation) of biologically and chemically-relevant mono-, di-, oligo-, and polysaccharides using various molecular modeling-based methodologies, including quantum mechanics methods, molecular dynamics simulations within classical, atomistic force fields, and coarse-grained modeling. In particular, the research involves the interpretation of measurable parameters inferred from NMR spectroscopy.

II. Development of Enhanced-Sampling Computational Methods

This area of research involves the development, testing and validation of classical force fields operating at both atomic and coarse-grained resolution. Additionally, existing advanced sampling methods applied in molecular dynamics simulations (the so-called enhanced-sampling methods) are improved, and new ones are developed. This work results in the development of coherent methodologies that enable more efficient and accurate simulations of diverse molecular systems.

III. Modeling Degraded Nanoplastics

Under the influence of solar radiation, temperature, and mechanical forces, plastic waste fragments into increasingly smaller particles, ultimately reaching the nanometer scale. These nanoparticles, commonly known as nanoplastics, exhibit different chemical properties in comparison to the source materials. The aim of the research is to computationally model the formation of nanoplastics and their further interaction with biologically-important species. The research stages include: modeling the chemical degradation processes of molecular materials from plastics; analyzing and classifying the generated surface functional groups; analyzing the interactions of degraded nanoplastic particles with blood plasma proteins; and analyzing the influence of surface functional groups on the processes of nanoplastic penetration through lipid membranes. Such simulations allow for the assessment of the scale of the nanoplastic threat to living organisms and enable a better understanding of the related phenomena at the molecular level.