

Krystalochemia i chemia obliczeniowa w badaniach oddziaływań niekowalencyjnych w polimerach koordynacyjnych oraz związkach o znaczeniu biologicznym =
Crystallochemistry and computational chemistry in the investigations of noncovalent interactions in coordination polymers and biologically relevant compounds

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In the article, we present some of the research topics being pursued by the Structure and Dynamics of Macrosystems research group. We try to connect experimental findings with theoretical description providing new knowledge and understanding of processes at molecular level. Using a variety of theoretical methods, we explain and supplement the results of experiments. Crystal engineering is a branch of science developing rapidly over the past few years. Based on this, we can design and control the crystal formation process, and thus obtain a structure with the desired physicochemical properties. Here, we show how crystal engineering has been combined with computational chemistry using as an example three-dimensional (3D) coordination polymer (CP) CuI/CuII of mixed valence $\{[\text{Cu}_3(\text{C}_{14}\text{H}_8\text{N}_3\text{O}_2)_2(\text{H}_2\text{O})_2](\text{BF}_4)_2\}_n$ with 2-(pyrazin-2-yl)quinoline-4-carboxylic acid as a linking ligand obtained based on solvothermal synthesis using Berghof reactors. Another interesting issue is an application of molecular dynamics in ab initio and classical schemes to describe molecular features of compounds with hydrogen bond. Usually, we perform simulations in the gas phase, with liquid or in the solid state depending on the project and therefore computational setup. A few years ago, we decided to study dynamical properties of the hydrogen bonds in one of the polymorphic forms of naphthazarin. We combined static quantum-chemistry approaches with Car-Parrinello Molecular Dynamics (CP-MD). The combination of various methods allowed a detailed description of the proton dynamics in the hydrogen bridges. From the beginning, in the research group we perform investigations of biologically relevant compounds/macromolecules. We focused on selected quinolone carboxylic acid derivatives, because of their

biological potential and possible practical applications as well as because of the various kinds of the intramolecular hydrogen bond present in the set of the studied compounds. Based on the obtained results, we were able to draw conclusions of the time-evolution of the hydrogen bridges and their influence on the molecular properties. The last topic, which we would like to introduce in the article is an application of the classical molecular dynamics to study extremophilic proteins. The search for examples of differences in the dynamics and structural properties of mesophilic and thermophilic proteins led to molecular dynamics (MD) simulations for a protein fragment from the bacterium *Caldanaerobacter subterraneus* subsp. *tengcongensis* (formerly *Thermoanaerobacter tengcongensis*) with a type 3 fibronectin domain (FN3) structure. Nowadays, the area of research seems to be very interesting and challenging therefore we put an effort to understand and explain some dependencies in such organisms to provide new knowledge useful in the design of new proteins with particular biological preferences.

Słowa kluczowe

crystallochemistry, computational chemistry, coordination polymers, naphthazarin, quinolone carboxylic acid derivatives, extremophilic proteins

krystalochemia, chemia obliczeniowa, polimery koordynacyjne, naftazaryna, pochodne kwasu chinolonowego, białka ekstremofilne

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