Hydrogen bonds in Shape-Memory Polyurethane Copolymers – a quantum chemistry study.

Description for the general public

What is common between a food package, medical stitches and an aircraft? All these examples contain or are completely made up of *polymer materials*. Such a wide comparison clearly shows how many different possible usage polymers have. Actually, an enormous number of already developed and potential applications have arisen due to different combinations of polymers named *copolymers*. Copolymers are materials that contain fragments of several different polymers, which is why they can be used in a greater number of ways. It is obvious that copolymers' applications are directly related to their properties. Features of the polymer used as the main material in the food package are for instance stiffness, non-toxicity and thermal resistance. However, copolymer qualities are not limited to mentioned examples.

Sometimes, even a bit "magical" nature of the copolymer can be observed. How about copolymers, that are capable of *remembering the shape* they obtained after production? You might be able to change their shape under specific conditions, and it will be stable. But when you apply the same conditions again, you will see, that the polymer recovers its original shape. This property gives a possibility to manipulate the shape of the polymer by manipulating external conditions. This is extremely important for example in medicine or aerospace industry, where the temporary shape allows to introduce the copolymer-based tool to the appropriate place and then "activate" by forcing it to shape recovery. The most impressive applications of shape memory polymers (SMPs) can be found in medicine, as smart scaffolds, vascular stents, smart-nerve-conduits, and in aerospace, as a material for self-deployable solar arrays, or sunshields, and even the potential "morphing aircrafts" with the ability of wings to adapt their shape to current conditions.

Although the exact mechanism of this property is not completely explained there are assumptions on the structural criteria necessary for polymers to have shape memory. First, these systems should contain 'switches' – specific structural fragments interacting in a special way. Second, they should be two-segmented, which is why in most cases those are copolymers. In addition to that, segments of SMPs should be separated on a micro level, in other words, the microphase separation should occur, so that each segment plays its role without the interruptions of another. The degree of such separation is controlled by interactions between segments: stronger interactions result in a higher degree of microphase separation. As the characteristics of these interactions strongly depend on the chemical composition of SMPs, an extensive study should be performed to establish and understand the correlation between the chemical structure of SMPs and the level of microphase separation.

Experimental research works are very informative: the results of experimental measurements and observations provide essential knowledge about the studied copolymers. The relationship between the structure and chemical composition of copolymers with their properties is mainly derived from experiments. However, such methods are not always successful in explaining obtained observations on a smaller scale, taking into account chemistry and physics of interactions we are interested in. This is where computational methods, which use theoretical knowledge and approaches to calculate the properties of the system, come into play.

Taking into account the need to investigate the interactions between segments of different compositions and the power of computational methods, this project aims at describing a particular type of interactions, namely hydrogen bonds, in shape memory polymers with the help of theoretical methods. Created model systems will be divided into three groups, and within each group the chemical composition of models' fragments will be varying. Computational chemistry methods will be further applied to analyse the strength and reorganisation of the interactions between particular segments. This information will allow to specify the microphase separation degree of studied systems. Model systems of project tasks are combined into a bigger system in the last project task. In the same way, the methodology applied for each task ends up in multiscale modelling methods in the third part of the project. A thorough analysis of obtained results will lead to a comprehensive explanation of the main aspects of microphase separation in terms of interchain interactions and the chemical composition of SMPs.

Concluding, the analysis of shape memory copolymers, conducted in this research, will provide valuable information about interactions in these copolymers, widening the current knowledge about key aspects of shape memory mechanism.