Study of dynamics in the interaction networks of selected co-crystals

DESCRIPTION FOR THE GENERAL PUBLIC

In a common knowledge crystals are solid and stable materials, which are one of the most durable forms of matter in the world. Their multiple symmetric forms as well as great variability of colors and kinds have always delighted humans, who considered them valuable. The dynamic science development and X-ray diffraction discovery at the beginning of the 20th century, enabled the visualization of the internal periodic structure of crystals. Since then, the scientific importance of the crystalline materials was only growing. In the middle of 1950s for the first time the term ‘crystal engineering’ was used by R. Pepinsky. He suggested that it is possible to control the crystal symmetry by proper choice of crystallized components. Immediately the question appeared: **How to select the chemical agents to get the expected results?** In the last few decades, this apparently simple inquiry has induced the development of the entire new branch of crystal studies.

Now let’s go back to the crystal nature. According to crystal diffraction properties, they are known to be a periodic and ordered type of solid matter. Such features can lead to the conclusion that crystal nature is stable, and therefore static. However, there could be nothing more wrong! In fact, all atoms and molecules within each crystal vigorously oscillate. Their movement is not chaotic and random. The molecule motions are conditioned by the symmetry of interactions of entire crystal structure. If we try to imagine such internal motions within the crystal we can associate it with some kind of complex dance. Each type of the molecule have its characteristic steps (interactions), which strongly depend on its environment. Their spacial arrangement – crystal self-assembly – is a result of set sequence of movements of all molecules within the system – the choreography. Here the two questions asked by the proposed project arise: **How to teach the molecules to dance with each other?** and **How to establish and plan their choreography within the crystal at particular conditions?** In fact, they are both a paraphrase of the question referred in the previous paragraph.

The answer to both questions can be partially found in the understanding of already mentioned ‘molecule steps’. However, such knowledge is insufficient. You don’t understand the choreography by learning steps. You do it by constant step practicing, dynamically, within the music rhythm, and with other people on the dance floor. In the project such practice is proposed in two-pronged approach. The theoretical approach will be based on the quantum-chemical method – the Born-Oppenheimer molecular dynamics – used to simulate the vibrations of molecules within the crystal. Within the project such computations will be performed for co-crystals – the specific type of multi-component materials. Co-crystalline systems are composed of multiple different molecular and/or ionic compounds. Because of their specific ability, which enable combining physical and chemical properties of co-crystallized components, co-crystals find multiple applications in the production of pharmaceutical and modern multi-functional materials. The simulation of dynamics, complemented with the interaction analysis based on DFT methods will improve the understanding of co-crystalline system self-assembly. Additionally in the second, experimental part of the project, a new polar and chiral co-crystals will be engineered and obtained. Their interaction networks will be investigated by the means of X-ray diffraction and spectroscopic methods.

To summarize, the proposed study is dedicated to augment the understanding of intermolecular interaction dynamics within the co-crystals. In addition, planned experiments can result in new co-crystalline systems, with prospective applications in the advanced optoelectronics.