

Photonic devices play a unique role in modern technology development. Light modulating systems, OLEDs, photorefractive devices, optically switchable molecular machines, photochromic lenses, biochemical probes and sensors are only a few examples of optical materials applications. Advances in optoelectronics require simple, stable and preferentially low-cost solutions. Efficient optical materials can be engineered for a specific application using quantum crystallography approach. This method is a combination of quantum chemistry computational tools for the purpose of understanding, characterization and engineering of crystalline materials.

In this project we will focus on new crystalline materials exhibiting large birefringence, high refractive index, substantial second harmonic generation (SHG, frequency doubling effect) and/or displaying chromic effects (stimulated colour change). The enhanced properties of a crystal can be obtained by incorporating two different building blocks in one crystal structure (cocrystallisation). First component has sufficient electronic properties (e.g. large hyperpolarizability) and a second one is ensuring proper orientation of the components to maximize the optical effect.

Crystal structure of new materials will be obtained from single crystal X-ray diffraction experiments. Experimental and theoretical electron density studies will contribute to the understanding of arrangement of the molecules in the solid state. Optical properties will be calculated using quantum mechanical methods (Q-LFT) and determined experimentally. Stability of the crystals will be examined using PXRD, DSC and TG methods. The proposed research project is expected to result in a number of new materials with substantial optical effects. The proposed research methodology will contribute to the understanding of structure-property relationship in the solid state multicomponent materials.