Multicomponent organic materials are of major interest in materials science because of their multiple applications in optoelectronics and information processing. Organic solids are known for their enormous optical effects and shorter response times to commonly used inorganic crystalline phases. When designing functional optical materials often it is necessary to obtain a crystalline phase with proper symmetry. For example, Second Harmonic Generation (SHG) effect, which leads to frequency doubling of incident light is observed only for noncentrosymmetric solids. Additionally, for remarkable optical effects, the electronic properties of crystal building blocks must be considered. The usage of molecules with large values of (hyper)polarizability, an ability to form electric dipoles in response to the external electric field, must be considered. Unfortunately, often molecules with large (hyper)polarizability are oriented antiparallel in crystal structure what can cancel out some optical effects. This issue can be overcome by introducing a second component to the crystal structure, which will maximize desired optical effects.

The aim of this project is to design and obtain new multicomponent optical materials containing sulfonamide and sulfonic acids. The sulfonyl derivatives were chosen as valuable components in materials design because they are easily accessible and scientifically examined. There is a large amount of data useful in crystal engineering of new materials. There are also multiple sulfonamides and sulfonic acids with a high value of (hyper)polarizability. The rational design of functional crystalline phases will be based on quantum crystallography approach. This branch of crystallography focuses on studying materials by a combination of structural information and quantum mechanical theory. The quantum crystallography tools will allow for quantitative and qualitative analysis of intermolecular interactions present in a crystal structure. The understanding of influence of interaction on molecular assembly in crystal structure will be used to obtain materials with tailored properties. The proper arrangement of molecules in a crystal structure will maximize optical properties of the material. The refractive indices, linear birefringence and SHG efficiency of obtained crystal phases will be determined. The correlation of mutual arrangement of molecules in the crystal structure with the magnitude of optical properties will be also ascertained.

The project's workplan will consist of following stages: design and preparation of new materials, crystal structure determination of obtained crystalline phases, determination of optical properties and analysis of intermolecular interaction using quantum crystallography tools for selected materials. The final stage of the project will be devoted to determine structure-property relationship.

The results obtained during this project will broaden the knowledge concerning the rational design of functional materials. The conclusions drawn from the structure-property relationship will be of key importance for crystal engineering of new materials with tunable properties.