The global increasing energy demand and depletion of natural resources are strong motivations for better exploitation of the available energy supplies and the development of new energy sources. Thermoelectric materials and devices are related to ecological energy sources due to the possibility of converting waste heat into electricity or vice versa. Only one independent parameter which strongly affects the thermoelectric performance of materials is lattice thermal conductivity. Finding a way to interlink thermal transport with crystal structure aspects is crucial for designing novel materials with ultralow lattice thermal conductivity for thermoelectric energy conversion.

The investigation of the crystal structure and thermal transport properties in close-packed tetrahedra (TCP) structures (filled-β-Mn-type and argyrodite-type compounds) shows that lone-pair-like interactions, bonding inhomogeneity, and structural disorder presumably appear as the main reasons for their ultralow lattice thermal conductivity. However, the evident interlink between these phenomena and thermal transport in TCP members is still not established.

In this project, we aim to find a relationship between structural and thermal transport properties of promising thermoelectric materials based on Cu_6Te_3S and $Cu_{9.1}TeSb_3$ with a close-packed tetrahedra structure. Particular attention will be dedicated to the effect of the crystal structure and chemical bonding analysis on the thermal transport properties of these promising thermoelectric materials. Moreover, such discovery should suggest more chemical reasons for the prediction of low lattice thermal conductivity in crystalline solids.

To solve these problems the following objectives will be accomplished:

- Systematic investigation of the crystal structure properties of the Cu_6Te_3S and $Cu_{9.1}TeSb_3$-based materials and analysis of chemical bonding between atoms.
- Investigation of the electrical and thermal transport properties in Cu_6Te_3S and $Cu_{9.1}TeSb_3$-based materials.
- Searching for the new crystal structure reasons, which are mainly responsible for the thermal transport in all studied close-packed tetrahedra structures for prediction of materials with low lattice thermal conductivity.

We hypothesize, that bonding inhomogeneity in Cu_6Te_3S and $Cu_{9.1}TeSb_3$-based materials can be mainly responsible for the low lattice thermal conductivity. Effective bonding engineering will help to suppress thermal transport and attune the electronic properties towards the high thermoelectric performance in the investigated materials. The use of advanced experimental and theoretical techniques will uncover the origin of ultralow lattice thermal conductivity in close-packed tetrahedra structures, including Cu_6Te_3S and $Cu_{9.1}TeSb_3$-based materials as well as filled-β-Mn-type and argyrodite-type compounds.

Due to the complexity of the crystal structure of TCP structures, crystal structure refinement will allow us to find possible ways for its modification to control the physical properties. Moreover, the accurately refined crystal structure would permit us to understand the origin of the thermal transport properties of the studied compounds and perform optimization of chemical composition to improve its thermoelectric performance.

We believe, that during project realization we will discover new chemical descriptors of materials with ultralow thermal conductivity. Moreover, the final conclusions of the project will help us to take a step further in the chemical understanding of electronic and thermal transport in functional materials.