The chirality phenomenon plays remarkably important role in the world around us. It is often observed, that one enantiomeric form of given pharmaceutic exhibits intended therapeutic effect, whereas the second one might appear harmful. Due to the necessity of obtaining chemical compounds of certain handedness, new methods of synthesis as well as of selective enantiomers separation are searched for. The cheapest and the easiest way of enantiomers separation from racemic mixtures is by crystallization. However, not in all chemical substances spontaneous chiral crystallization is observed. What is more, mechanisms and rules behind this phenomenon are not fully recognized. Crucial role in mutual recognition of molecules of given chirality plays intermolecular bonds, among others hydrogen bonds, van der Waals interactions or electrostatic interactions can be distinguished. New class of compounds, in which all of the most significant interactions types may be found are ionic co-crystals built of both organic and inorganic components. What is more, by rational design it is possible to obtain structures of intended molecular architecture.

In ionic co-crystals structures of lithium salts a chain-like coordination polymer built from chiral six-membered fused rings is very often observed. The aim of the project is to analyze the impact of selected factors on this base building block structure and thus to determine results of such changes on superior levels of molecular architecture up to consequences in macroscopic crystal chirality. This research may contribute to understanding of structural mechanisms behind spontaneous chiral crystallization. The analysis will be possible thanks to specially designed, big enough structural library - a coherent data set - where main architecture will be preserved and only chosen parameters altered. To obtain structural library lithium halides and biogenic amino-acids will be used. The basis of the project will be single crystal X-ray crystallography experiments followed by meticulous data analysis supported by theoretical methods such as periodic calculations or graph theory.

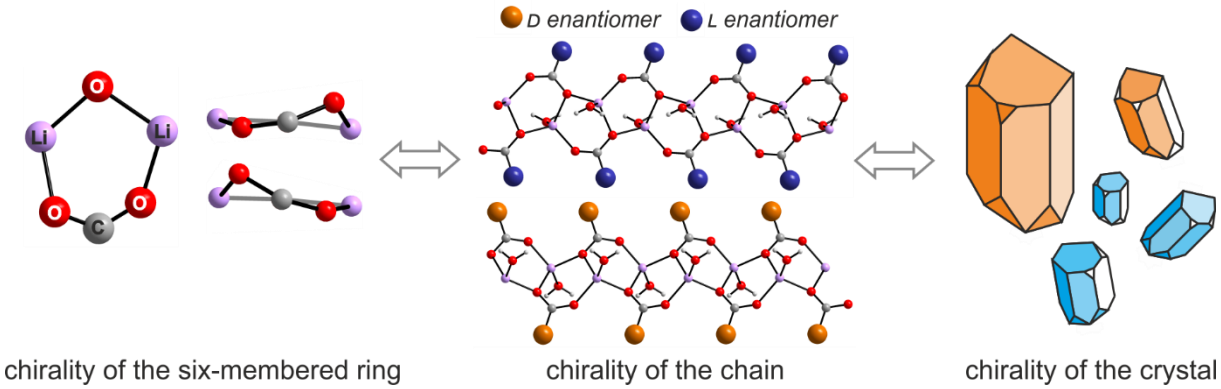

Figure 1. Levels of chirality observed in ionic co-crystals of lithium halides and amino-acids.