

Atoms and molecules in crystals move about their equilibrium positions and sometimes far from equilibrium positions. Crystals behave as collective ensembles of many-many molecules that can reorient, move, isomerize and react showing us how living matter emerges from chemistry and how to design artificial systems with new properties.

In the frame of the proposed project we would like to explore dynamic properties of the molecular crystals with flexible architecture responding to cations and anions. Such flexible molecular crystals are quite rare, but promising for applications in separation, sensing, catalysis and host-guest chemistry. We perceive the flexibility of such architecture as its ability to attain a large number of accessible structural states while retaining crystallinity. We plan to induce structural transformations by the addition of cations and anions under very mild conditions implementing crystal soaking methods. Soaking is the process of taking pre-grown crystals and soaking them with the small molecule of interest. After that the crystals are subjected to the single crystal X-ray analysis, providing determination of the positions of all atoms in the studied crystal. This allows us to visualize the binding sites for cations and anions in the native framework and the corresponding structural change of architecture. We hope to answer question how can small molecules and ions permeate the crystals? What kind of intermolecular interactions facilitate ion transport through the pores? What is the role of water molecules filling the pores in the process?

The fabrication of flexible molecular crystals responsive to ions and small molecules is important for many reasons. Such crystals are expected to exhibit *solid-state activity*, necessary to act as chemical sensors, separators and ion reservoirs. They potentially can act as crystalline membranes or crystalline sponges operating in water-based media.