

### **Project 3.3. Ion permeation in the molecular crystals**

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**ICP PAS Group:** Team 22: Charge transfer in biological systems and at the interfaces

**www:** <http://groups.ichf.edu.pl/zarzycki>

#### **Background:**

Nowadays we are witnessing the maturity and bloom of crystal engineering and its going hand-in-hand with the supramolecular chemistry. This fruitful marriage paves the way to the design and synthesis of artificial supramolecular crystalline solids exhibiting various dynamic phenomena, such as swelling, breathing, guest transport, solid-state reactions, to name a few. The proposed project will be oriented towards exploration the dynamic behaviour of the molecular crystals based on the charge-assisted hydrogen bonding and host-guest interactions. Such crystals are supposed to adapt to different auxiliary guests/ions by regulating molecular conformation and assembly mode of its building blocks. Instead of actively explored conventional porosity that requires the harsh activation and preservation of the open structure, we would concentrate on the permeability and guest binding in the pores of molecular crystals. To achieve this we are going to implement crystal soaking approach widely used in biological crystallography. The crystals will be analysed by X-ray single crystal diffraction to reveal the binding of auxiliary guests in the pores and corresponding structural response of the native framework. The PhD student will have the opportunity to realize part of the project tasks in University of Bologna (Department of Chemistry) during planned foreign fellowship.

#### **Aim:**

The aim of the project is to explain how the interplay of hydrogen bonds, ionic forces and host-guest chemistry allow the formation and subsequent structural transformations of the permeable molecular crystals. We hope to answer question how can small ions and/or molecules permeate the crystals? Would some new interactions emerge facilitating ion transport through the pores? What is the role of water molecules filling the pores in the permeation pathway?

#### **Requirements:**

- master degree in chemistry or related field;
- good command of English;
- knowledge/experience in the field of X-ray crystallography, supramolecular chemistry.