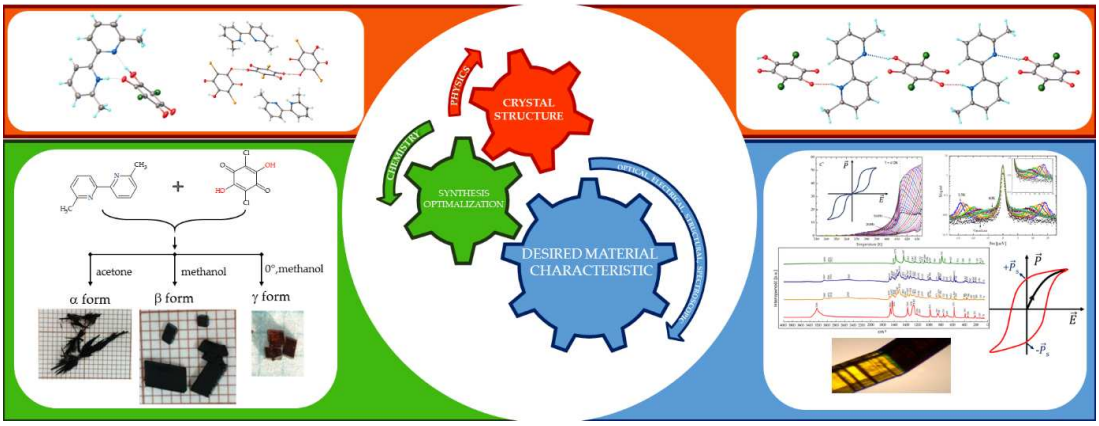
Structure *versus* antiferroelectric and semiconducting properties of the aromatic base/acid complexes and organic/inorganic hybrids

Organic ferroelectrics with asymmetric hydrogen bonds X–H···Y are the most promising dielectric materials for applications in organic electronics. An increased interest may by associated with: (*i*) the manner of their preparation - usually such functional materials can be obtained from the simple synthesis of two compounds from solution; (*ii*) the fact that they can be easily deposited and patterned by inject printing; and (*iii*) the most important idea, that organic materials can be a good alternative to toxic inorganic oxides containing lead, bismuth, tantalum or niobium. **The main goal of this project is to design new functional materials for a possible application in organic electronics.** As well as, we would like to focus on the correlation between crystal structure and physical properties of materials such as ferroelectricity, antiferroelectricity or protonic conductivity and even semiconductivity. Out research project will focus on (**i**) organic complexes based on the organic aromatic amines and acids and (**ii**) organic-inorganic hybrids (ionic type) with a general formula $R_aM_bX_{(3b+a)}$ (where R- organic cation of methyl-derivatives of pyrazine, M = Sb(III), Bi(III) and X = Cl, Br, I). The investigations of the novel materials that exhibit a very large polarization value, which may be useful in capacitors and nonvolatile memories, can be discovered in systems proposed in this project.



In conclusion we can state that in a synthesis we plan to use a pair of molecules (not exploited up to now in literature), which are promising from the viewpoint of the interesting physicochemical properties. Especially we are looking for organic crystals exhibiting structural phase transitions leading to **antiferroelectric and/or semiconducting phases**.

The research objectives are as follows: **1.** Synthesis of several organic complexes containing simple aromatic bases and organic acids or inorganic units; growing up their single crystals. **2**. Determination of their crystal structures. **3**. Detection of the structural phase transitions and a determination of dynamical properties of the crystals. **4**. Studies on the electrical properties of crystals (dependence of electric permittivity over the wide temperature and frequency range, the temperature dependence of electric conductivity, *dc* and *ac*). **5**. Conclusions on a relationship between crystals structure, mechanisms of the structural phase transitions and dynamics of proton in the hydrogen bonds. **6**. Explanation of an effect of hydrogen bonds strength on appearance of such properties like ferroelectricity, antiferroelectricity and semiconductivity. **7**. Elaboration of the theoretical model parameters on the basis of the experimental data (Havriliak–Negami relaxation, Ising theory and mean field theory).

The team has an adequate scientific potential and research background to undertake the research in the framework of this project. Synthesis, single crystal growth and basic physicochemical investigations will be carried out in laboratories of the Faculty of Chemistry University of Wroclaw. Some measurements will be performed under collaboration with the other centres – Institute of Low Temperature and Structural Research of the Polish Academy of Sciences in Wrocław, Institute of Molecular Physics PAS, Poznań, calculations will be carried out in Wroclaw Centre for Networking and Supercomputing.