The main objective of the project is the design and synthesis of new so called metal-organic framework materials (MOFs) with proton-conducting property (so called PCMOFs) based on innovative, environmentally-friendly and cost-effective mechanochemical approach. Another objective is to determine the structures and physicochemical properties of the obtained materials. This objective extends also to the determination of a correlation between conducting properties and the structures of PCMOFs.

Metal-Organic Frameworks (MOFs) are among the most exciting developments in nanotechnology to emerge in recent years. Constructing MOFs by chemists can be compared to building with block-toys, composed of sticks and balls, by children. Using 'chemical' balls and sticks one can create a MOF with crystalline structure which resembles a molecular scaffolding (or sponge) and consists of metal ions (balls) linked by organic molecules (sticks). The combination of these components produce materials with a variety of desirable properties such as eg. nanoporosity, high surface areas and thermal stability. Nanoporosity of these materials means they possess open space that can be filled with other molecules, called guests. One of the ideas in this project is to build MOFs whose pores can be filled in such a way that it will make the MOFs electrically conducting. Conducting MOFs are currently an emerging field of research. The conduction means charge transport through MOFs and in this project it is understood as proton (positive charge) conduction. It can be for instance imagined as a proton hopping on parts of the molecular scaffolding. Such proton-conducting property can have profound implications for the future of various sensors, energy conversion and storage. In particular, proton-conducting MOFs (PCMOFs) can be used as essential parts of fuel cells that generate electricity by a chemical reaction producing harmless water. Apart from interesting MOF materials and their properties, in this project it is also planned to use environmentally-friendly and cost-effective mechanochemical methods to synthesize the aforementioned PCMOFs. These methods rely on exerting force on molecules. In particular, the targeted novel materials are expected to be obtained on the way of solid-state grinding of reactants. Apart from ecology, this method brings low cost and ease of manufacturing, key sought-after factors in terms of applications and large-scale use in many technologies.

The research proposal includes four main research tasks. The first major research task is the design and synthesis of the targeted PCMOF materials. This task includes two parallel strategies: i) a two-step post-synthetic mechanochemical modification of so called dynamic MOFs and ii) direct one-step mechanosynthesis. The second research task will be the screening of all solids obtained immediately after grinding. For this purpose, it is planned to use mainly X-ray diffraction and infrared spectroscopy. These methods will allow for the identification of pure products and their selection for further structural and proton conduction investigations. The third research task is the determination of the composition and structures of the obtained new MOFs. For this purpose, it is planned to use mainly X-ray diffraction with numerous analytical and spectroscopic techniques. Determination of the composition and structure of the obtained MOFs is necessary to understand its correlation with physicochemical properties, including proton conductivity. The fourth research task in the project will be the determination of physical and chemical properties of the obtained MOFs. For this purpose, it is planned to carry out mainly electrical measurements. These measurements will provide the information about conductivity values, its dependence on selected parameters, and the mechanism of the conduction. For PCMOFs with determined structures, the key molecules forming a conduction pathway are also expected to be identified.

The financial support of this project will create a unique know-how of MOF materials and this knowledge can be patented. The results obtained within this project will be published in well-recognized international scientific journals and will be presented at national and international scientific conferences. MOF materials, proposed in this project, have enormous practical applications, and thus affect the development of civilization. In particular, a promising is the new emerging subclass of proton-conducting MOFs (PCMOFs), being the crux of the project, and with a potential for application in fuel cells technology. The resulting solution (developed synthetic pathways towards PCMOFs) or product (obtained compounds and the research findings for those with appropriate conducting properties) can be transferred to the chemical industry, for example to the fuel and energy sector, and then they will affect the development of civilization and societies.

In summary, this innovative research project simultaneously combines three extremely important and highly topical areas of modern chemistry (three-in-one):

1) Metal-organic framework (MOF) materials which can be compared to scaffoldings built from molecules;
2) Mechanochemical synthetic methods ie. through exerting force on molecular scaffoldings; and
3) Proton-conducting properties that are useful for sensing, energy conversion and storage applications.