It has been know for decades that properties of matter is strongly affected by pressure. It strongly transforms the minerals inside Earth and other planets. The mechanisms of these processes are still not fully understood, and in many cases not accessible for our learning. An example of the effect of pressure is the synthesis of the diamond, which is the hardest known material indispensable for industrial and technological applications. High-pressure production of synthetic diamonds generates profits worth billions. Can this success be repeated? Unfortunately, our knowledge about the effects of pressure is still insufficient in many areas of physics and chemistry. However, owing to the invention of the diamond-anvil cell, more and more subtle high-pressure effects can be now investigated in scientific laboratories.

Pressure effect on porous materials belong to the most fascinating subjects. There are many such materials in Nature. Commonly known are zeolites, porous aluminosilicate minerals commonly used as commercial adsorbents and catalysts. Silicate zeolites can be also synthesized and mimicked by porous metal-organic frameworks (MOFs) with properties similar to zeolites.

Preliminary high-pressure studies showed that MOFs exhibit exceptional physical and chemical properties. The compression of MOFs strongly depends on the framework of organic ligands and their connections. Most of crystals interact with environment with the surface of their walls and it is thermodynamically required that they shrink at high pressure. MOFs additionally interact with the surface of their pores – it is very large and for one gram of the compound it can be comparable to the football pitch. Consequently, the components of the environment can penetrate the pores and affect their volume. Some molecules can interact with pores stronger than others and be selectively adsorbed from around. This property can be employed for isolating specific compounds and for eliminating air from green-house gases (carbon dioxide, methane), poisonous (carbon monoxide, hydrogen sulfide) and for storing energetic gases (hydrogen, methane). These properties would be welcome by the motor industry and environmental protection. Selective isolation of MOFs includes also chiral compounds and in pharmaceutical applications MOFs can be used for administering regular doses of drugs to patients.

It was shown in recent years that high pressure can be advantageous for the properties of porous materials. In particular, it was shown that pressure efficiently affect the organic linkers and the structure of the pores in the pores. This in turn considerably changes the response of MOFs to external stimuli. For example, in high pressure not only the positions and inclinations of the ligands can be considerably modified, but also the coordination of the metal ions changed. These and other contributions can combine into exceptional deformations of MOFs in extreme conditions. For example, the rare negative linear compressibility (when the crystal extends in one direction in increased pressure) as well as extremely rare negative area compressibility (when the crystal section area increases) have been observed. MOFs can be also ferroelectric and ferromagnetic, and can be applied in sensors, opto-electric transducers and absorbers of vibrations and shocks. However, it still remains most essential to understand the effect of pressure for making the full advantage of the exceptional properties of MOFs.

The primary aim of the envisaged grant will be the synthesis of MOFs and the study of their transformations at high pressure. The project will consist of several tasks: (1) the syntheses of MOFs; (2) determination of their structure and positions of guests in the pores; (3) analysis of the interactions responsible for the adsorption of the guests; and (4) the construction of high-pressure devices optimized for the specific requirements of the investigations of MOFs. All results will be published in the form of scientific papers in the international journals and patents.