Design and synthesis of multifunctional composited based on metal-organic frameworks and organic polymers for small molecules separations

Metal-Organic Frameworks (MOFs) are porous coordination polymers consisting of inorganic (metal node) and organic part (organic linker). Almost unlimited possibility to create new structures allows to design their composition and properties towards specific applications. Their tunable pore's sizes, shapes and chemical environments allow rational design towards efficient sorption and separation systems.

The composites based on MOFs and organic polymers are nowadays intensively investigated. The research area concerning with the preparation of mixed matrix membranes (MMMs) is especially intriguing and is based on uniform distribution of crystalline MOFs through amorphous polymer. The proper choice of the organic polymer can enhance the stability of the whole system, and moreover change its properties (e.g. increasing hydrophobicity). The preserved porosity of those composites is especially important for their separating applications. The current challenges in preparation of MMMs include nonuniform dispersion of used constituents and the possible blockage of MOF's pores due to the uncontrolled polymer growth.

The proposed research project concerns with a design of a new two-step strategy of obtaining MOFpolymer composites. In our approach, the organic polymer will be directly coordinated to the metal node (Fig. 1). In a first step, the post-synthetic functionalization of selected MOFs is performed to incorporate radical initiators. Obtained in this way functionalized material will be in a second step used to initiate radical polymerization reaction of selected monomers introduced into its structure. We expect that this original approach will allow us to control the length of growing polymer chains in a MOF structure (Fig. 1, I-III). The most promising composites will be tested in separation of challenging mixtures, (for example, mixtures of hydrocarbon isomers or Xe/Kr). Depending on the final chemical properties of the prepared systems, additional studies will be performed concerning water purification from heavy metals or biologically active molecules.



Fig. 1. Scheme of the designed strategy of preparing MOF-polymer composites. In a second row, controlled filling of the pores of MOF with growing polymer chains directly coordinated to the inorganic nodes