Description for the general public

Nowadays, the need for a far-reaching approach to the subject of energy, both in the aspect of energy sources and ways of its storage and conversion, is particularly felt in the international arena. In the near future, one of the most promising direct sources of electricity, converting it from chemical energy, will become fuel cells, particularly those using hydrogen as a fuel. If a green hydrogen source is used, the cell will become a completely climate neutral source of electricity, with heat and water as the only byproducts of its operation.

Metal-organic frameworks (MOFs) are hybrid organic-inorganic materials with extremely fast-growing chemistry. Almost unlimited possibilities of their design and porous characteristics predispose them to be candidates for many applications in science and industry, including energy-related industries. For several years, MOF materials have been sought to meet the challenges posed by designers of gas storage facilities (e.g. for hydrogen storage), by designers of fuel cell electrodes, or of proton-conductive membranes. There are already many reports in the literature in which metal-organic frameworks have shown desirable properties in each of the aforementioned structural parts of hydrogen fuel cells.

Within this project, comprehensive research will be undertaken on the application of a selected category of chemical reactions: the inverse electron demand Diels-Alder reaction (iEDDA) as an example of a very mild and efficient method for the covalent post-synthetic modification of metal-organic frameworks to introduce or improve their proton-conductive properties (Figure 1).

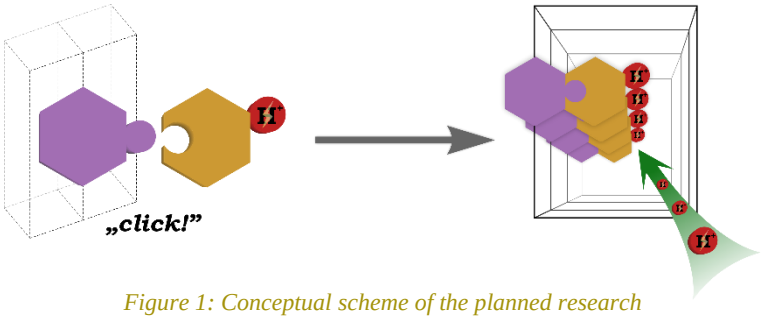

Figure 1: Conceptual scheme of the planned research

A key problem facing researchers designing MOF materials for use in the construction of proton-conducting membranes is the difficulty of introducing proton donors and acceptors that would be the source and carrier of the charge transported in the solid electrolyte. Despite the high synthetic potential of MOFs and their inherent porosity, obtaining material with a free acid or base group is problematic due to the tendency of such groups to coordinate with forming nodes. A circumvention of this problem is the use of post-synthetic modifications that introduce a donor or proton carrier after MOF assembly.

Within the planned project, research will be conducted on selective introduction of certain functional groups by means of the iEDDA reaction. It should be noted that so far there are very few examples of the use of this reaction to modify metal-organic frameworks, and there is not a single literature example of application of any click reaction (cycloaddition) to introduce/improve proton-conductive properties in any materials. This fact further strengthens the motivation to undertake research on the indicated topic. An additional motivation is the fact that the incomparable selectivity of this reaction may enable the precise introduction of a certain number of functional groups into specific sites of the crystal structure, and the mildness of this reaction may enable monitoring of these modifications by X-ray structural techniques.

The achievement of the intended research goal is planned through the realization of six research tasks including the design and synthesis of ligands (Task 1), MOF materials (Task 2) and dienophiles (Task 3), performance of covalent post-synthetic modifications (Task 4), fundamental physicochemical characterization of the obtained MOF materials (Task 5) and proton-conductivity studies using electrochemical impedance spectroscopy (Task 6). The planned research tasks will mostly be carried out in the professionally equipped laboratories of the Coordination Chemistry Group of the Faculty of Chemistry of the Jagiellonian University in Krakow, by the PI. Some of the planned tasks, in particular the preparation of precursors of MOF materials with particular chemical stability and advanced adsorption analysis of responsive and flexible materials will be performed in cooperation with the centers of ICMol (Valencia, Spain), TU Dresden (Germany) and the University of Bergen (Norway). The realization of the project will enable the implementation of a universal method for introducing and improving the proton conductivity of MOF materials, regardless of their initial durability.