"Metal-Organic Frameworks for catalytic CO_2 conversion"

The atmospheric concentration of carbon dioxide (CO_2) has been rising extensively since the Industrial Revolution and has now reached dangerous levels, contributing to the climate change.
Direct transformation of the abundant CO_2 to valuable chemicals and fuels is currently of great importance from the viewpoints of environmental and green chemistry. The inert nature of CO_2 limits the number of transformation methods, so it is important to develop the effective catalytic methods for converting CO_2 by low energy input. CO_2 can be used as a feedstock for production of organic cyclic carbonates (OCs), dimethyl carbonate (DMC) or methanol (CH_3OH) (Fig.1). All of those products are used as substrates in chemical and pharmaceutical industry.

For example, cyclic carbonates are used as chemical intermediates, polar solvents, electrolytes in lithium ion batteries, coatings, additives to cosmetics and detergents and can be obtained e.g. by the cycloaddition of CO_2 to epoxides or carboxylation of diols. Among these methodologies, cycloaddition of CO_2 to epoxides has been the most investigated because it is considered to be a green process. However, epoxides are highly reactive and most of them is toxic. The alternative, green method of OCs production can be carboxylation of diols obtained e.g. from biomass. This reaction yields only OCs and H_2O.

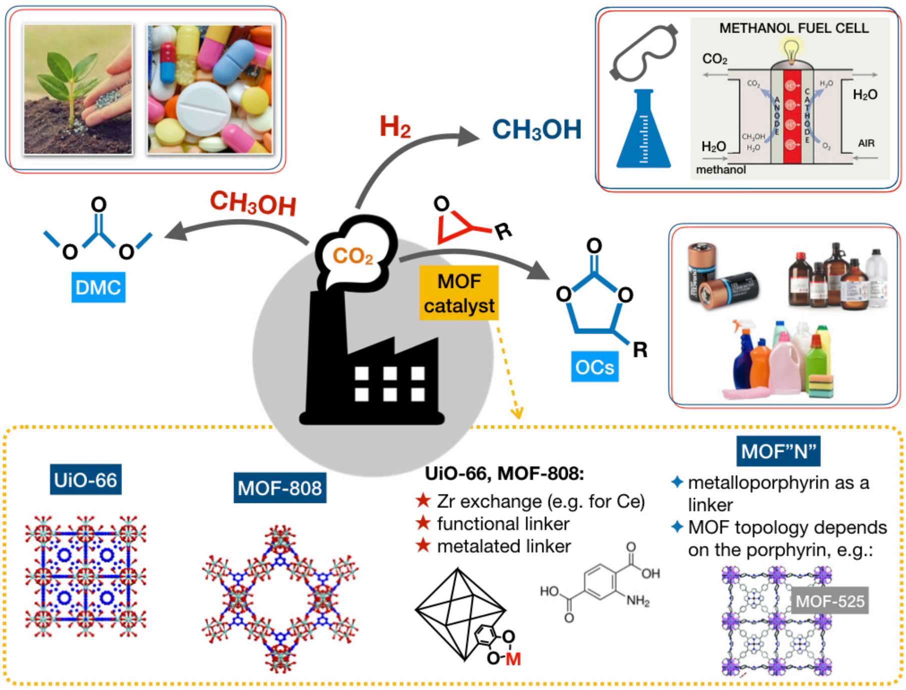

Figure 1. The idea of the project – CO_2 conversion to valuable chemicals using MOF catalysts.

The catalysts used for CO_2 cycloaddition to epoxides are metal oxides, zeolites, transition metal complexes, quaternary ammonium salts, ionic liquids and Metal-organic frameworks (MOFs). Owing to crystalline nature, chemical tunability, remarkably high surface area and regular pore structure, these materials seem to blend some of the best features of the homogeneous and heterogeneous catalysts.

The main objective of the project is to develop active and stable MOFs for converting the abundant CO_2 to other products such as cyclic carbonates, dimethyl carbonate or methanol. The synthesised MOFs will be bifunctional, i.e. will contain two types of active sites: acidic (for the activation of epoxide, methanol or H_2) and basic (for the activation of CO_2).