Reg. No: 2021/41/B/ST4/00048; Principal Investigator: prof. dr hab. Kinga Góra-Marek

Each process in the world takes place on an individual time scale. There are processes that occur within fractions of a second and those whose duration can be counted in decades or even centuries. Although the duration of a given reaction seems to be its strictly defined parameter, it is not invariant. There is a broad range of substances that can significantly prompt chemical reactions, biological processes and, above all, industrial processes. They are called catalysts; in their presence, the process running naturally over many years can be finished in several minutes. The phenomenon of catalysis, first described in 1836, is now the most dynamically developing fields of science. The practical importance of catalysts is illustrated by the fact that about 90% of the products of the chemical industry are obtained through catalytic processes (mainly heterogeneous catalysis).

Searching for new catalysts and a detailed description of those already recognized is a challenge for a huge number of scientists. The catalysts based on porous crystalline materials, such as zeolites or metal oxides, are of particular interest. The material aspiring to be an active catalyst have to possess numerous active sites, i.e. the places where direct contact with the reactants takes place. The selectivity is also of great importance. We are interested in the production expected reaction product as the only one. The catalyst has to be also stable and as cheap, if possible.

It is not possible to design new catalysts without a comprehensive characterization of both the currently working catalysts and the materials that are just up for that title. Catalytic activity, i.e. the ability to is inextricably linked with the catalyst's active sites. Therefore, a comprehensive description of all the catalyst's characteristics has been an area of research for many years. Although a qualitative description of the active sites is necessary for the understanding of the catalytic process, it is still not sufficient. Only the combination of the qualitative picture with quantitative information can fully illustrate the catalytic process. The project implementation meets the challenge of researching real "working conditions" of an active catalyst, with the use of reagent molecules, i.e. in the so-called *operando* mode. Such an approach will not only complete the picture of the active sites' properties but will also enable the monitoring of changes in active sites occupation by individual species of a chemical reaction.

IR and UV-Vis spectroscopies are powerful tools that allow conduct not only gualitative but also guantitative monitoring of the catalyst surface. However, the registration of the spectra of the catalysts itself is useless if the reactant molecules are not bound on their surface. As part of the project, an innovative IR-Vis-UV approach is proposed to use a single spectrum collected within the entire IR-Vis-UV range in the same moment of the catalytic reaction. The measurements will be carried out in the time-resolved mode (rapid scan), enabling the registration of the spectrum in 0.1-1 s. Correlating these two spectroscopic techniques under the catalyst operating conditions (operando) with the measurement of the catalyst activity and selectivity (GC analysis and mass spectrometry) allows determining not only the global speciation of the active catalyst's sites but also visualizing the actual course of the reaction, which usually takes only fractions of a second! These studies will be supported by a correlation analysis: the 2D spectra will allow us to conclude about the order of events in the catalytic nano-world. This research is unique. So far, there are only a few literature reports on the use of 2D COS IR spectroscopy to study catalytic processes. So far, the development of this methodology towards using the ultraviolet to infrared radiation range to study any phenomena occurring on the surface of the zeolite nanocrystals has not been proposed yet. The processes we will investigate are oxidation reactions with the use of atomic oxygen produced by the decomposition of N₂O or O₂ molecules. Apart from the economic aspect, the investigated processes are important for environmental protection. With their effective use, we can control the emissions to the atmosphere of harmful nitrogen oxides and volatile organic compounds.

The idea of this project was born from the necessity to develop the methodology of quantitative research dedicated to active sites in the real working catalyst which provides knowledge on the mechanisms of many catalytic processes. It opens the door, for designing not only cheap and effective catalysts but above all, the catalysts dedicated to specific processes.