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The individual time scale of all processes occurring around the world around can be noticed. There are known processes lasting only fractions of a second and those which duration can be counted in the years, decades or even centuries. Although the duration of the process seems to be strictly well-defined parameter, still it is not invariant. There is a wide range of substances that are able to significantly shorten the duration of many chemical reactions, biological processes and, above all industrial processes. Catalysts, because about them we discuss, do not directly participate in the process but still they significantly shorten its duration; thus processes extending over many years can be completed in a few minutes. The phenomenon of catalysis, first described in 1836 by Swedish chemist Jons Berzelius, is now the core of one of the fastest growing areas of science. The practical significance of catalysts can be illustrated by the fact that about 90% of chemically derived industrial products originate from catalytic processes (mainly heterogeneous catalysis). The searching of new catalysts and a detailed description of these already identified drawn the attention of broad scientific community. Especially popular are catalysts based on porous crystalline materials such as zeolites or metal oxides. Decades of research on zeolite catalysts and oxides revealed the existence of several important aspects of those materials the must be fulfilled in order to be considered as a catalyst in for instance petrochemical industry. Pretender to the title of an effective catalyst must possess in a structure the active centers where the direct contact between the reactants and the catalyst occurs. Furthermore, the porous structure of the zeolite or the oxide grains must present mutually intersecting channels and chambers allowing easy access of molecules reagents to active centers. The attention is paid also to the fact that the catalyst should be durable, economic and highly selective, thus allowing to obtain the maximum amount of the expected reaction products.

Design of new catalysts is not possible without a thorough characterization of both those currently used as well as materials only aspiring to that name. The catalytic activity, being a measure that allows to assess the accelerations of the reaction or process, is directly linked with its type of active centers. Therefore, the obtaining of their complete characteristic has been for many years an area of scientific research interest. Although the qualitative description of the active sites, allowing for determination of its type, is necessary to understand the catalytic process, it is still insufficient. Only a combination of this information with quantitative image allows to fully illustrate the process. Quantitative studies of active centers, due to the degree of difficulty and its problematic nature are extremely rare. Therefore, the primary objective of this project will be an attempt to develop new, and above all simple and effective methods of quantitative analysis of active centers. Project investigators also planning to meet the challenge of conducting research in a real "working conditions" of active catalyst using conventional processes, ie. in the so-called operando mode. This approach not only fulfill the image of properties of the active centers, but also allows for monitoring the changes occurring in active centers as well as particular individuals concentrations during course of chemical reaction.

IR spectroscopy is a powerful tool for performing, not only qualitative but also quantitative analysis of the properties of the active sites. The most valuable information from IR spectra about oxides and zeolites cam be withdrawn if their surface will be covered by probe molecules. The IR bands appearing in the IR spectra are in fact the result of the bond vibration in probe molecules interacting with the active sites. The studies proposed in this project concern the use aa probe molecules both the commonly used species such as ammonia, pyridine, carbon monoxide(II) and nitrogen oxide(II) as well as the most important reagents of the catalytic processes. IR measurements will be carried out with use of the classical spectrometer and the one that allows for considerably faster scanning of spectra (so-called Rapid Scan method). Correlating those two techniques of collecting the spectra allow to determine not only the comprehensive image of the centers of active catalyst, but also will depict the actual course of the reaction, which usually takes only fractions of a second! Despite the undeniable advantages, IR spectroscopy has unfortunately some limitations; thus it not allows to clearly distinguish between all types of active centers, including the acidic type as well as those associated with the cations of transition metals. However, methods such as Raman spectroscopy, or UV-Vis spectroscopy, allow to specify the type of active sites by detecting the form in which a transition metal occurs (eg. a form of exchangeable cation or oxide). In order to complete the picture, the materials will be investigated under the reaction conditions representative for SCR NOx, SCO NH3 and VOC elimination in which usefulness of the proposed quantitative research methods and mechanism of catalytic reaction itself will be verified.

The idea of this project was born from a desire to increase knowledge of the quantitative studies of the active centers of various types. The fulfillment of the basic tasks of the Project, which is developing a relatively simple and effective tool for conducting quantitative characterization, allow to fully understand the mechanisms of many catalytic processes. Moreover, it will open the gate, through which it will be possible to design not only cheap and effective catalysts, but above all, catalysts dedicated to specific processes.