Karolina Tarach *Untangle Spectroscopic Results of Heterogeneous Catalytic Systems*

The spectroscopic picture of the catalytic reaction in heterogeneous systems is extremely complicated because it is a composite of many spectra coming from a very large number of reactants participating in this process. In each of these processes, you can find both reagents actively participating in the course of the reaction and those only accompanying it, not affecting the selectivity of the process. In order to be able to observe them, it is necessary to conduct the reaction in laboratory conditions in a way that is as close as possible to how it actually takes place in the industry. These conditions are called "operando". In order to best identify the processes occurring during the reaction, many techniques are used simultaneously to characterize the catalyst surface as well as the reaction products. However, to determine with certainty which of the reactants are the active ones and which are only the accompanying "operando" measurements are not sufficient. Only the appropriate modulation of the reaction system, e.g. by changing the concentration of one of the reactants (Modulation Excitation Spectroscopy, MES), and the simultaneous examination of the concentration of all other reactants makes it possible to detect those that are actually active and not only accompany the reaction. The results collected from many such experiments and then mathematically transformed (Phase Sensitive Detection, PDS, and Multivariate Curve Resolution by Alternating Least Squares, MCR-ALS) will serve for the identification of active reactants of the catalytic reaction. This, in turn, will allow for better design of the catalyst so that it exhibits higher activity and selectivity. A good choice of the available research methods is infrared spectroscopy, as it enables measurements within the time-scale of the phenomena that we want to observe. The main goal of the project is to develop a toolbox that will help us to untangle the complex spectroscopic picture of the catalytic system and to distinguish important active reactants from those merely accompanying reactions.