There's no doubt that olefin metathesis is one of the most important chemical reactions discovered in the twentieth century and investigated during the last decades. Many various chemicals having versatile applications can be synthesized in this way, what's important, also on industrial scale. One of many examples of olefin metathesis application is selective production of propene. One might therefore conclude that the metathesis reaction is already well known and further work on this process should not be a mainstream research. Nothing can be further from the truth than this. It turns out that despite many years of studies on olefin metathesis, some fundamental questions are still being debated.

One of the most pressing problems is the determination of the surface species in the heterogeneous catalysts for olefin metathesis. These catalysts are solid substances capable to perform the metathesis reaction. In particular, the questions concern active centres, i.e., that piece of the catalytic system that directly takes part in the process. Besides, the mechanism of the formation of these centres is not determined as well. From the standpoint of the new catalysts designing, answers to these questions are fundamental in nature. Without this knowledge, the searching for new highly active catalysts is like wandering in the dark. So far, the experimental studies of existing catalysts produce rather inconclusive results. So, that's why in this project it is planned to prepare new catalysts, in an innovative way. We expect that these novel catalytic systems should be more suitable for experimental characterization. For the first time it is planned to apply a variety of different, advanced spectroscopic methods, in combination with molecular modelling. It should allow to explain the mentioned above issues related to heterogeneous olefin metathesis catalysts.

In large-scale chemical processes based on olefin metathesis reactions, predominantly heterogeneous catalysts are used. They are basically composed of a transition metal oxide (usually Mo or W) deposited on thermally stable support of a high surface area. However, many factors significantly influence catalytic activity, among them the method of preparation is of particular importance. First of all, the type of the support used significantly affects the catalytic activity, although this effect has not been fully explained. An interesting alternative to the traditional supports appears to be the use of mesoporous materials with ordered pore structures. These materials have numerous advantages. Due to the regular arrangement of the pores and their relatively large diameters, the access of the reactants to the internal surface inside the pores is facilitated. It usually results in a higher catalytic activity. Therefore, one of the main aims of this project is to develop and synthesize novel heterogeneous catalysts for olefin metathesis. They will contain molybdenum and tungsten oxide supported on mesoporous materials with ordered internal structure. The modifications of acidic properties of the systems studied by adding heteroatoms to the structure of the support can significantly affect the catalytic activity.

It is generally accepted that the metathesis reaction catalysed by heterogeneous systems occurs according to the carbene mechanism. It is assumed that at the beginning of the reaction, during the initiation stage, the alkylidene species ($M{=}CR_2$, wherein M is a metal atom and R is a hydrogen or alkyl group) are formed as a result of an interaction between the olefin molecule and the surface oxide precursor. The metal oxide precursor is the phase on the support formed during the catalyst preparation, not being metathesis active yet. Only the alkylidene species are those that directly catalyse metathesis reactions. However, the mechanism of the formation of the alkylidene species is not determined. Moreover, the structure of the metal oxide precursors and the alkylidene species is not determined as well. Therefore, the planned researches in this field seem to be fully justified.

In this project, comprehensive investigations of the mechanism of olefin metathesis catalysed by heterogeneous molybdenum- and tungsten-based systems is planned. To do this, determination of the surface species structure is necessary. It will be done based on various experimental *in situ*/*operando* methods, including Raman spectroscopy, FTIR and UV-Vis. *In situ/operando* techniques allow to perform direct and continuous measurements of the catalyst surface during the process. Hence, the information received from these techniques are very helpful in the study of mechanisms of catalytic reactions.

Complementary information can be obtained using computational methods of quantum chemistry. The still growing computational power enables to study systems with increasing complexity and reliability. In this project, it is planned to perform computer simulations of large systems using density functional theory (DFT) approach, a powerful tool of theoretical chemists, which will provide the additional knowledge about the examined surface forms. This knowledge will enable the next step, in which the attempts to explain the mechanism of the initiation stage of olefin metathesis process will be made. We are going to verify the reaction mechanisms proposed in the literature, but it is also possible that the calculations will indicate a new, so far unknown mechanism. This part of the research will be carried out using molecular modelling. The propagation stage will be studied as well.

It is expected that the final results of the project able us to explain the influence of the metal (Mo or W) and support nature on the catalytic activity for the initiation and propagation stages of the olefin metathesis process, as well as to determine the mechanism of the active sites formation.