Chemical catalysis is the increase in the rate of a chemical reaction due to the participation of an additional substance called a catalyst. The use of a catalyst yields faster reactions and/or lowers the temperature needed for the reactions to take place. As a result, catalytic reactions are preferred in environmentally friendly green chemistry due to the reduced amount of waste generated and power and/or time consumed. The production of most industrially important chemicals today involves catalysis.

From the chemical point of view catalyst lowers the free energy barrier of the reaction, meaning that less free energy is required for the substrate to reach the transition state. Catalyzed reactions have a lower activation energy (rate-limiting free energy of activation) than the corresponding non-catalyzed reaction, resulting in a higher reaction rate at the same temperature and for the same reactant concentrations. In most cases the detailed mechanisms of the action of catalysts are complex and catalysis is often a multi-step process. Obviously there are no universal catalysts, but each chemical reaction can be catalyzed by a unique catalyst.

The main goal of this research project is a systematic study of selected chemical catalysts directed toward better understanding of the fundamental aspects of their action. Within this project we plan to design and perform modelling studies of new ruthenium-based systems able to catalyze an important chemical reaction: metathesis. This task will be carried out in an interdisciplinary, multinational team consisting of scientists, experts in carbene synthesis, experimental ruthenium-catalyst preparation and analysis and rational design and modeling of transition metal complexes. The results of this project will allow for an accurate characterization of a series of new carbenes and complexes and allow to develop a general methodology, which will be used in the future to design new, better catalysts.

The focus on the olefin metathesis reaction is justified, as this reaction has been named as "emerging green technology" by the Royal Academy of Science during the 2005 Nobel Prize award and was quickly adopted by research groups as a basic strategy for the synthesis of carbon-Carbon bonds. The ability of this method for the selective substitution of atoms between two molecules allows the generation of chemical systems with the desired properties. This is particularly important for complex compounds such as natural compounds and new heterocyclic compounds and macrocyclic compounds. The use of cross-metathesis, ring-opening and ring-closing metathesis and acyclic diene metathesis polymerization allows the synthesis of compounds via simpler pathways and starting from cheaper raw materials. The development of novel complex architectures for investigated reactions should make a significant scientific impact.

The overwhelming number of applications of metathesis reaction nowadays is truly remarkable, especially considering the short time since it was first observed. A large number of olefin metathesis applications in various industries have been growing over the years. The synthesis of numerous complex organic molecules and materials, such as pharmaceuticals, polymers, agrochemicals and natural products, has been facilitated by well-defined catalysts. Despite the wealth of accumulated research, there has been an ever increasing academic interest in this area over the years. Most current efforts focus on finding new applications, answering some elusive questions regarding the mechanism, and improving catalysts through systematic tuning of their properties. This is also the scope of this proposal – to expand our knowledge about this interesting class of compounds.

This project will also strengthen research in Poland and Germany. We hope that this project will increase the competitiveness of Polish in the field of chemical synthesis and catalysis, and its results will be useful to the polish and international chemical community in better understanding the relationships between structure and reactivity of selected catalysts. It is also a pitch for stronger collaboration between these countries, their two prominent academic institutions and three scientific groups with related interests. Within the timeframe of this project we will create vital, international synergies between three scientific groups working in closely related fields to further advance the chemistry of catalytic systems based on ruthenium. One of the goals of this project is also to immerse a number of young scientists in a world-class science, by giving them the opportunity to work on this project. The expected result of this collaboration is the development of new skills of these young scientists and the opportunity to broaden their horizons in a multi-national environment.