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. Nowadays, the production of most industrially important chemicals involves catalysis and similarly, most biochemically significant processes are also catalyzed.

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 important chemical reactions: metathesis, hydrogenation, transfer hydrogenation and hydrosilylation. We will also develop new computational methods to accurately describe catalytic processes not only at the atomic level but also at the nano/mesoscale level. These tasks will be carried out in an interdisciplinary team consisting of scientists specializing in organometallic chemistry, rational design and modeling of complexes, catalysts and physics. The results of this project will allow for an accurate characterization of new catalysts and allow to develop a general methodology, which will be used in the future to design new catalysts with desired properties. The long-term goal of the project is the appointment of a new research team which will provide expertise in the fields of computational catalysis and create vital synergies with experimental groups working in the field of organic/inorganic synthesis and catalysis.

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. 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. The broader goal of this research is to expand our knowledge about carbenes and its analogues and advance the field of organic catalysis and strengthen Polish potential in this field. The long-term goal of this project is to incorporate computational and modeling tools into organometallic research to obtain a new methodology for rational design of catalytic compounds with desired properties.