The main scientific aim of this project is to determine the mechanism of oxidative dehydrogenation (ODH) of lower alkanes (such as ethane, propane and isobutane) over catalytic systems containing the active vanadium phase introduced into matrix of porous materials.

Within the project, in the first step, the heterogeneous catalysts structured of beta zeolite and well-defined vanadium centers will be synthesized. In the nest stage, the physicochemical and catalytic properties of the prepared catalysts will be examined and correlated with the results of quantum-chemical calculations. The catalytic systems, mentioned above, will be exhaustively investigated in the important, from practical point of view, reaction of oxidative dehydrogenation of lower alkanes to alkenes. Parallel to experimental studies, the quantum-chemical calculations will be performed in order to find and determine the mechanism of ODH reaction depending on the used alkane and structure of active vanadium site. The investigations which are planned to be carried out within this project are important both from scientific and practical point of view. The planned dual fundamental studies (experiment and theory) will give insight into the role of the relevant physicochemical properties of the catalysts (e.g. synthesis method or structure and nature of active sites) and parameters of ODH reaction (e.g. reaction temperature, composition of reaction mixture); these studies enrich the knowledge of catalysis. On the other hand, elaboration and explanation of the ODH reaction mechanism using efficient and well-defined heterogeneous catalysts gives real possibility to obtain desired alkenes in more economically and environmentally way than by catalytic cracking of heavy fractions of crude petroleum.