Description for the general public

One of the main challenges for the practical chemistry is the optimisation of methods of fuel production from reasonably available sources. In principle, the transformation of one substance into desired product is almost exclusively possible in the presence of a catalyst, able to direct the reaction. Liquid fuels are being produced by petrochemical industry where zeolites are the mainly used catalysts. Zeolites are crystalline porous aluminosilicalites which can be either found in natural deposits or synthesized. The pores in zeolites create unique systems while they cross each other forming caves. Moreover, extremely strong acidic sites, even stronger than mineral acids, can be localised in the zeolite structures. Besides Brønsted acidic sites the metal cations can be introduced becoming the redox sites. Variety of structures, pore sizes, available cations which can be introduced together with a number of ways of zeolite modification build up enormous potential for application as well as for fundamental research. The knowledge how to influence the geometry of zeolite during or upon synthesis together with controlling of the formation of the sites allows for the design and synthesise modern (high-tech) catalysts. However, the intentional directing synthesis of zeolites is possible when the deep understanding of the rules and factors important for mechanism and chemical transformation inside the pores is achieved.

The main goal of this project incorporates a variety of experimental methods (IR spectroscopy, transmission electron microscopy, roentgen diffractometry) as well as computational methods which, for many years, are recognised as very successful, will be used for research of zeolite structure.

The computational methods of chemistry offer the methods to describe both the elementary steps of chemical reactions at atomic and molecular level and also to describe the macroscopic systems. The combination of those methods is the second key issue of this project. The theoretical studies corroborated by experiments are excellently complementary in such way that the experimental results constitute the constraints for the computational modelling while the theoretical simulations of the elaborated model predict the results of the other experiments which in turn can be experimentally verified confirming or falsifying the postulated model. It can be stated that the contemporary computational methods, especially describing the chemical world at the atomic scale can be regarded as new experimental method and its application in scientific research keep growing dramatically.

Within the submitted project the planned study comprise the influence of the kind of active site in zeolite on its activity and selectivity and also the influence of the arrangement of pores of one kind on the speciation of active sites and their accessibility for the reactant molecules. It will be important to decide the influence of the channel arrangement on the reactant diffusion and on the kind of the chemisorbed complex formed. The applicability of the computational methods combined with the experimental techniques in the fully qualitative methods of study of the physicochemical processes in the multiscale form. The localisation and the kind of the active sites as predicted by quantum-chemical methods will be studied.

The results will be the basis of the doctoral theses of the PhD students for whom the members of the project team will be the scientific advisors.