Reg. No: 2015/19/P/ST4/02482; Principal Investigator: dr hab. inż. Izabela Czekaj

The urgent needs for a more sustainable production of chemicals from renewable feedstock (e.g. biomass) have caused intensive research efforts in search for novel porous nano-materials such as zeolites. The catalysts are still discovered through a combination of trial-and-error and serendipity due to limited understanding of molecular structure and complexity of active centers. The main goal of the project is design at nano-scale zeolite with improved catalytic performance, optimized for biomass transformation to dedicated chemicals. The research will focus on the zeolites with different pore size. The zeolites, commercially available in purely microporous form, will be prepared also in mesoporous shape and with addition of selected metal nanoparticles. In the project new insights from both molecular modelling and experimental methods will be used to obtain knowledge about zeolite topology and catalytic properties. The project will bridge molecular modelling and experimental tools to obtain complementary knowledge about zeolite catalysts topology. The integration of both paths, experimental and theoretical, in the same team is a novel approach and guarantees rapid progress in new catalysts and processes development as well as exceptional training for students in the subject of nano-design of zeolite-based catalysts for selective conversion of biomass into chemicals. The realistic three dimensional models of zeolites with added internal metal nanoparticles will be designed. In the proposed research subject variety of unresolved problems and uncertainties exist, whose solution will have a significant impact on the development of science and economy of zeolite catalysts design and production for environmentally friendly production of important chemicals. Development of catalytic routes for the conversion of bio-renewable feedstocks to selected key petrochemicals is expected. Examination of effect of the zeolites as support on nanostructure and reactivity of the metal nanoparticles will be. Role of zeolite structure will be studied on reactivity in biomass conversion reactions: the isomerization, dehydration, hydrogenolysis. Active sites and electronic structure of zeolite catalysts during reactions will be explored, which will lead us to development new class of catalysts with declare molecular structure. It is expected that new insights from both virtual modelling and experimental tools will make it possible to determine proper nano-scale design of zeolites with improved catalytic performance, optimized for biomass transformation to dedicated chemicals. Furthermore, it will bring knowledge into the real potential of zeolite as an essential tool in biomass conversion.