Basicity and metal are the key-factors for many common reactions in the catalytic processes of biomass transformation like alkylation, addition, condensation or hydrogenation [1]. These reactions are usually carried out in the liquid phase with the application of homogeneous catalysts. Using basic liquid catalyst requires the neutralization of post-reaction mixture, operating at relatively low temperatures, employment of base-tolerant reactor and supply of fresh catalyst portion in every cycle [2]. Heterogeneous catalyst can eliminate those issues, optimizing economically a process, however, designing effective catalyst is still a challenge due to leaching of active phase and need of its regeneration before each reaction cycle.

Glucose is an easily available biomass source that can be processed and transformed into fine chemicals and further to biofuels [3]. One of the possible paths of glucose transformation is fermentation which occurs over bacteria and gives as products mixture of acetone, butanol and ethanol (ABE). ABE can further undergo alkylation leading to renewable alternative transportation fuel components production [4]. The aim of the project is to design metal-base heterogeneous catalysts efficient for the liquid-phase reaction of alkylation of butanol with acetone as a model reaction for biofuel production.

Proposed in this project catalytic materials are core-shell nanostructured mesoporous silica, where core and shell can be separately functionalized, exhibiting various features. Therefore, the idea is to introduce basicity in the form of magnesium oxide nanoparticles in the core, while a metal in the outer shell and investigate active phases separation effect that enables following the desired diffusion pathway of the reaction sequence. Moreover, localizing basic sites in the inner core should prevent it from leaching to the liquid phase. Two factors related to the catalysts are going to be investigated: 1) distance between the base and the metal corresponding to the catalyst structure, 2) metal kind with the focus on low-cost transition metals as copper (Cu) in comparison with ruthenium (Ru) catalytically active according to literature. The mesoporous character of used silica support is expected to provide easy flow of reagents and accessibility to active sites. The influence of each factor on catalytic activity will be examined by a parallel study of suitable reference samples.

Catalysts are going to be characterized by several advanced analytical techniques in order to investigate the efficiency of planned materials' synthesis. It is planned to measure textural properties, the strength of the basic sites and the oxidation state of introduced metals and find the correlations between these features. All mentioned factors are expected to have a direct influence on catalytic performance. Catalytic testing in the alkylation reaction will enable a selection of the most active catalyst. Further process optimization by adjusting reaction parameters (temperature, reaction time, amount of catalyst, etc.) will contribute to the production of the best results.

The described project gives novel insight into a generation of stable basic active sites in accompany of metal nanoparticles in the catalyst. It assumes a complex analysis of the nature of obtained materials and studies of their application in the reaction that is environmentally important in the sense of replacing crude oil derived fuels by biofuels.

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