POPULAR DESCRIPTION

Pollution of the environment, and in particular atmospheric pollution, belongs to one of the major harmful aspects of development of the modern civilization. Noxious gaseous impurities can yet be removed by means of suitable catalytic processes such as oxidation or decomposition (reduction), using various redox catalysts, i.e., the chemical system that allow a given reaction to occur in a cyclic way, without altering the composition and structure of the catalyst itself. It should be emphasized that the effectiveness of catalytic action depends on many factors, the full understanding of which, due to the complexity of the heterogeneous catalyst-reagent systems, requires extensive and in-depth experimental and theoretical investigations. Recently, catalysts based on nanometric oxides of transition metals have received particular interest, due to their high reactivity, earth abundance and relatively low costs.

The overall research purpose of this project is to provide a rational basis for regulating the redox properties of model transition metal oxides to control the course of catalytic reactions of small molecules that are involved in the O-O, N-O, C-O, C-H, O-H and N -N bond breaking and making events. Such processes are associated with environmentally important methane combustion, total and selective oxidation of carbon monoxide and decomposition of nitrogen oxides (N_2O and NO_x). These gases are harmful and/or contribute significantly to the greenhouse effect. Within this project, we will focus our interest on determination the main factors affecting the redox properties of the oxide catalysts in relation to their structure and electron properties that can be sensibly shaped by appropriate chemical doping and control of the catalyst nano-morphology.

Three transition metal oxide systems of increasing complexity will be proposed for the investigations. In the first step, the attention will be concentrated on a model Co_3O_4 system of controlled cubic and octahedral shape, the redox properties of which will be controlled by aliovalent doping with lithium and boron. The second group of catalysts is constituted by mixed transition metal oxides containing double redox pairs, whose optimization will allow to adjust their redox potential to the particular catalytic reaction of interest in this project.

Heterojunction catalysts, consisting of two types of redox oxides connected by a coherent inter-grain boundary, are structurally the most complex systems to be investigated. They will allow to determine possible synergistic effects of an interfacial stress and charge segregation along the borderline on the catalytic activity. In the final stage of the project extensive catalytic tests using selected catalysts that exhibit highest activities in methane combustion, total and selective oxidation of carbon monoxide, decomposition of N_2O in the presence of typical contaminants, and reduction of nitrogen oxides will be performed.

In order to accomplish the planned tasks and meet the objectives, complex interdisciplinary studies combining the synthesis of catalytic nanomaterials, their thorough physicochemical characterization by means of a wide range of spectroscopic, microscopic techniques, physical properties measurements and chemical reactivity studies are required. Experimental studies will be supported by theoretical computation of the selected catalysts structure, their interaction with the reactants and modelling the mechanism and kinetics of the catalyzed reactions.

The proposed project will provide not only a fundamental knowledge for designing of new catalysts, but also, in a broader perspective, practical hints for manufacture of oxide catalysts with improved properties, based on readily available earth abundant components.