Multifunctional elecrocatalysts for clean energy conversion (*MultiCat*)

In recent years, there has been growing interest worldwide in generating pure (green) hydrogen as an energy carrier and feedstock for the chemical industry. Hydrogen, produced by electrolysis using renewable electricity, is essential for a successful energy applications and for meeting international climate targets. Efficient generation of green fossil-free hydrogen at low cost requires intense studies and development of new materials and implementation of novel methodologies. The ***MultiCat*** project aims at the development of multifunctional technologically-advanced catalytic materials for efficient generation of hydrogen (at cathode) and simultaneous evolution of oxygen (at anode) gasses via electrolytic water splitting. The oxygen evolution reaction seems to be limiting factor during the electrocatalytic water splitting. In the proposed research, we are going to address the problem and accelerate the processes (particularly the oxygen evolution reaction) by considering transition metal (e.g. iron, cobalt, copper or nickel) phosphide nanostructures which are emerging as efficient catalytic materials and alternatives to the presently utilized very expensive noble-metal oxides, such as ruthenium oxide or iridium oxide. Furthermore, some of the prepared nanomaterials will be used as multifunctional catalysts for hydrogen evolution reaction. In this respect, transition metal carbides will also be considered as effcient cathode materials. Novel protocols for the preparation of catalysts, which are characterized by defined functionality and activity, will be based on combination of conventional wet-chemistry and solid-state chemistry techniques. The joint studies of collaborating groups from Poland (*University of Warsaw*), Austria (Vienna University of Technology), and Slovenia (University of Nova Gorica) will concentrate on the development and optimalization of activity of the proposed advanced catalytic materials containing intentionally generated structural defects through engineering of cationic and anionic vacancies. The catalytic systems will be dispersed and immobilized on various supports or carriers just to improve the systems' stability and their electrochemically active surface area. Having in mind the tremendous recent drive toward practical utilization of low-temeprature hydrogen-oxygen fuel cells in automotive industry, there has been continuous interest in development of electrocatalytic systems for the efficient oxygen reduction reaction. Here in ***MultiCat*** project, special attention will be paid to development of both noble-metal-free electrocatalytic materials for the oxygen reduction with the ultimate goal of lowering formation of undesirable H_2O_2 intermediate which limits performance fuel cells. New generation of single-ligand and mixed-ligand metal organic frameworks (*MOFs*) with extended electron conjugations will be synthesized and applied as catalysts in this respect. With the use of highly conductive ligands, a truly novel iron, titanium, and copper - containing *MOFs* with predicted enhanced electrochemical performances and stabilities will be developed. ***MultiCat*** project will also refer to computational guided studies (*density functional theory, DFT*) to develop catalytic systems with intrinsic defects. The complementary research skills of research groups involved in this project will lead to the development of efficient multifunctional catalysts of importance to hydrogen technology and the environmentally-friendly low-temperature electrochemical energy conversion.