DESCRIPTION FOR THE GENERAL PUBLIC

The technology utilizing fossil fuels to generate energy causes the emission of billions of tons of carbon dioxide per year. Although the emission is small compared to the total CO_2 emission of the Earth, it disturbs the natural balance between the emission level and the absorption of carbon dioxide by plants and the oceans. The continuous increase in carbon dioxide level in the atmosphere is observed for over 150 years, and is assumed to greatly contribute to the greenhouse effect.

The utilization of waste CO_2 that is emitted to the atmosphere has become one of the most important issues the science has to deal with. Because the CO_2 is a very stable molecule, the process requires energy input – preferably obtained from renewable sources. Nature deals with this problem by means of photosynthesis process, where CO_2 is being converted into useful chemicals – such as sugars – with the use of solar light as the energy source.

The process of the CO_2 reduction is of a complex and multistep nature. Several possibilities exist with respect to the products of this process, for example methane (CH_4) or methanol (CH_3OH) that can be used as the fuels or fuel components. In these processes at least one of the C-O bonds must be cleaved. Altenatively the H_2 molecule can be attached to one of the C-O bonds leading to the formation of the formic acid (HCOOH). Different catalysts show different selectivity - the ability to direct the reaction towards one particularly desired product. This proposal aims to explain the details of this process, including the reaction mechanisms and interactions between the reactants and the catalyst. This will lead to better understanding of the process and in turn will enable tailoring the catalyst to suit the particular needs.

The aim of this project is to build the artificial device, having a characteristics similar to natural leaves. The device will consist of two parts: One is the photoanode, which role is to extract protons and electrons from water molecules in a process driven by light. The other is a cathode, where the protons and electrons generated at the anode will be used to hydrogenate the CO_2 molecules. This device mimics the natural photosynthesis also in the fact that it separates physically the water oxidation (at the anode of the artificial leaf and at the photosystem-II in nature) from the CO_2 reduction (at the cathode of artificial leaf and by the RuBisCo enzyme in nature).

The goal will be achieved by the combination of two distinct approaches in the form of a synergy - computer simulations of the process will provide the valuable data regarding the reaction mechanisms and intermolecular interactions. They will also allow to understand the photoexcitation process. On the other hand - the laboratory experiments will confirm the theoretical results and will provide the necessary data about the exact structure of the catalysts, what will allow to create realistic simulation models.