ABSTRACT FOR THE GENERAL PUBLIC

Project title: *Shedding light on gold catalysts – Delving into the role of phosphate ions in shaping the catalytic performance of Au/FeNbO$_x$ nanocomposites in the photo-assisted oxidative esterification of benzyl alcohol*

It is impossible to imagine a modern world without catalysis. Estimates show that approximately 85 − 90% of products of the chemical industry are made in processes that involve catalysts. The phenomenon of catalysis lies in the acceleration of a given chemical reaction by lowering the energy barrier that must be overcome to initiate the process. Therefore, a catalyst is for the reactants what a bypass is for car drivers who want to avoid traffic jams passing through a big city. Most of the industrial catalytic processes (approx. 80%) are carried out in the presence of heterogeneous catalysts, that is, catalysts that are in a phase different from that of the reactants (e.g., solid catalyst *vs.* reactants in the liquid or gas phase). Such a system allows for easy separation of the catalyst from the reaction mixture after the process is completed and its reuse.

Furthermore, we can perceive catalysis as a pillar of *green chemistry* and a key tool for reaching the sustainability goals, set out in the 2015 UN resolution. For example, considering oxidation processes in the liquid phase, thanks to catalysis, we can eliminate hazardous inorganic oxidants, such as chromates or permanganates, which produce large amounts of toxic waste. In their place, catalytic processes involving more environmentally-benign oxidants, such as oxygen (O_2), can be used. Such oxidants, after transformation, produce water as the sole by-product. It is very important to seek environmentally friendly methods for alcohol oxidation processes because these reactions lead to key products (e.g., aldehydes, acids, or esters) being used, among others, in pharmaceutical, cosmetics, or food industries.

Since the ground-breaking discoveries of M. Haruta and G. Hutchings in the 1980s, heterogeneous gold catalysts have been attracting steadily growing attention of scientists. For ages, gold had been widely recognised as almost entirely chemically inert, until it turned out that this noble metal, in the form of well-dispersed particles (i.e., with dimensions in the order of 10^{-9} m), deposited on various supports, appeared to be a high-performance heterogeneous catalyst for oxidation processes. It is generally accepted that the catalytic performance of gold catalysts in these processes is strongly affected by the support properties. Among a wide array of possible supports for gold, mixed metal oxides have focused the attention of researchers because they exhibit unique properties when compared with those observed for the corresponding single oxides. Over the last decades, there have been many reports that indicate that the properties of gold catalysts can be modified with the use of phosphate ions, which often leads to an effective increase in the catalytic activity of the obtained composites.

The project aims at the **synthesis of new heterogeneous catalysts** containing **gold nanoparticles** supported on **phosphate-doped mixed iron-niobium oxides** (Au/P:FeNbO$_x$). The composition of these catalysts will vary in terms of the phosphorus content. The catalysts will be characterised using techniques that complement each other and are commonly used to analyse solid materials. Moreover, the catalytic activity of as-prepared materials will be studied in **visible-light-assisted oxidative esterification of benzyl alcohol using oxygen as an oxidant** (Figure 1).

Understanding the relationships between the type and properties of the active sites present on the surface of gold catalysts and the activity/selectivity of these catalysts in oxidation processes remains a significant challenge. Detailed analysis of the aforementioned relationships makes it possible to tune the composition of the materials in order to obtain efficient and highly selective catalysts. **The main goal of the project is to determine the most promising molar ratio P/(Fe+Nb), which will guarantee high activity, selectivity, and stability of the planned catalysts in the process of oxidative esterification of benzyl alcohol.** We expect that the implementation of this project will broaden the basic knowledge on the design of multifunctional materials for the catalytic processes of the conversion of alcohols into *fine chemicals*.

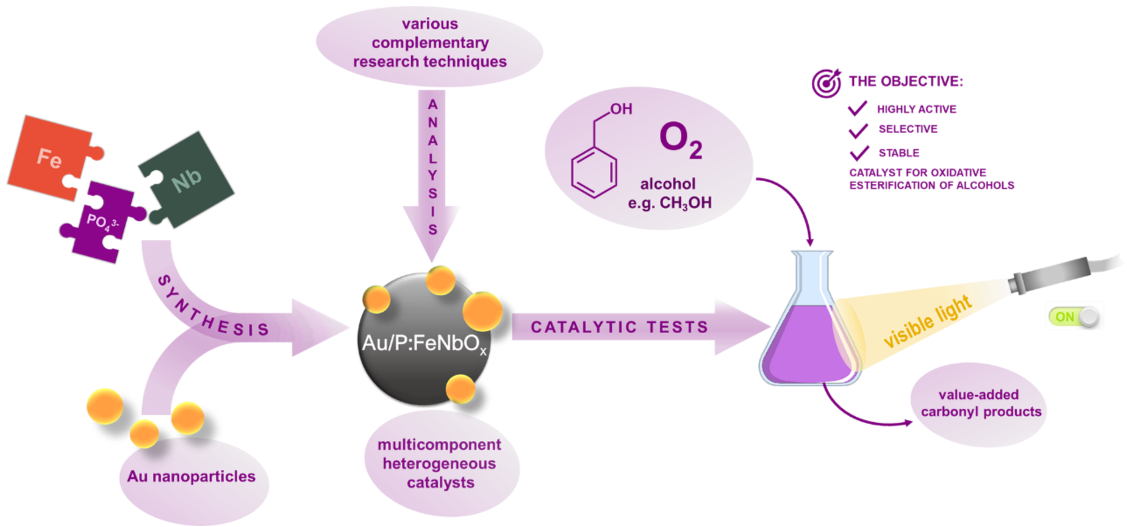

Figure 1. Schematic representation of the research project concept.