

Due to the constantly increasing human activity, water systems around the world are being exposed to more and more chemical contaminants such as pesticides, personal care products or heavy metals. This situation bears risks, both due to its scale and possible effects, and therefore, development of the new water treatment technologies are right now a global concern.

In this regard, heterogeneous photocatalysis have been proposed as a sustainable solution – a process where suitable semiconductor (photocatalyst) absorbs light and initiates redox reactions involving photoexcited electrons and holes. These reactions might lead to the formation of highly reactive oxygen species which are able to oxidize persistent organic pollutants. The only problem remaining is to find material that could provide sufficiently high process efficiency.

Therefore, the main goal of the proposed project is to look up for the strategy to increase photocatalytic activity of the photocatalysts utilized in the water treatment technologies. As a starting point, nanoparticles of the same photocatalyst's polymorph, but differing in its surface structure, were selected. This approach was based in the latest reports showing that atoms arrangement at the semiconductor's surface affects pathway and efficiency of the photocatalytic processes. This is a result of different charge carriers' behaviour, which might either localize on the surface atoms and efficiently initiate further reactions, or, due to their quantum mechanical nature, might delocalise over the bulk structure of the photocatalyst, which would severely limit their reactivity. Above all, this effect allows for the detailed insights and discussion about the mechanism of the photocatalytic reactions and because of this, it also offer an way to control the elementary reactions that initiates the whole process.

However, outside of the pure photocatalysts, the effect of their surface structure is little known, In this regard the interactions between photocatalyst's surface and introduced modifications will be systematically investigated in the project. The goal is to maximise the photocatalytic activity of the designed materials, as the combined effect of the surface structure, introduced dopants (affecting equilibrium charge carriers concentration), as well as deposited co-catalysts – another materials that contribute to charge separation by “pulling” the charge carriers out of the photocatalysts crystal structure.

The ability of the obtained photocatalysts to generate reactive oxygen species will be investigated in detailed both for pure and modified structures, which subsequently will be tested against the selected water pollutants. As a result, the Authors expect to find answers to some fundamental questions, such as a (i) *how does the photocatalyst's surface structure influence on the dopant effect when considering water treatment processes?* (ii) *how does the same surface structure interacts with other materials, introduced as co-catalysts?* (iii) *how does the obtained surface-modifications compositions affects photocatalyst's ability to generate reactive oxygen species?* and (iv) *how does all of this determine photocatalyst ability to degrade water pollutants?*