Data-driven materials design: Artificial Intelligence as a tool supporting the synthesis of nanocomposites with hierarchical porosity for electrocatalytic applications.

The demand for advanced materials for "clean energy production" is constantly growing and is associated with the search for safer, cheaper, and more ecological solutions. Among these sought advanced materials are compounds for basic processes of future technologies, including those with catalytic properties. Catalytic properties are understood here as those accelerating chemical reactions, among other things, by lowering its energy barrier, i.e., the barrier that must be overcome to initiate the course of the reaction. **In particular, researchers and industry practitioners are interested in materials that can be used for electrocatalytic reactions, i.e., those in electrochemical systems at the electrode/solution interface. One such electrocatalytic reaction is the oxygen reduction reaction (ORR),** an energy source in devices such as fuel cells, microbial fuel cells and metal-air batteries. Currently, the research on electrocatalytic processes is dominated by materials based on noble metals, such as platinum and palladium. However, they are characterized by low durability, susceptibility to gas poisoning, low activity and selectivity. The second group of materials popular in electrocatalysis is carbon materials with a large number of pores, in which the main limitations in achieving high operational efficiency are, among others, the heterogeneous structure of their surface, high content of impurities, low resistance to oxidation and inefficient transport of electrons and heat.

Motivated by these challenges, as part of the project, we plan to synthesize nanocomposite materials containing cyclic skeletons with nitrogen atoms in their structure and spherical carbon nanostructures (multi-layered fullerenes), which should be characterized by high electrocatalytic activity. This idea is unique because nanocomposites of this type have yet to be used in electrocatalytic reactions. Our research shows that nanocomposite materials have properties such as high electronic conductivity, a large number and increased accessibility of active sites for reactants, high porosity, which enables easy transport of electrons, and high chemical and electrochemical durability. As part of the project, we plan to design highly efficient nanocomposite catalysts with particular emphasis on the correlation between the porous structure of materials and the efficiency of the electrocatalytic reaction and to design advanced materials for electrocatalysis using the "lab-in-the-loop" approach based on artificial intelligence (AI). Our main goal is to revolutionize the synthesis methodology by developing an AI-based approach to catalyst design to improve the electrocatalytic performance of materials and achieve outstanding performance parameters.

Using only a synthetic methodology leading to achieving the goals set in this project is a very time-consuming, costly and tedious process. The use of organic synthesis tools to obtain many groups of new nanocomposite materials requires multiple repetitions of procedures (from several hundred to even several thousand different combinations), in which many variable parameters must be introduced, starting from different synthesis conditions. The possibility of combinations is endless because we should change one variable each time in the synthesis process to check which determines obtaining a material with the desired electrocatalytic properties. In addition, the obtained nanocomposites should be thoroughly characterized by specifying their physical and chemical parameters, which will translate into the selected electrocatalytic properties we intend to achieve.

As part of this project, **we intend to combine experimental work in obtaining materials for electrocatalysis with AI in the form of machine learning (ML) algorithms**. Using ML to find the relationship between the structural parameters of the substrate, product and electrocatalytic performance may favor the design of new systems with advanced properties. We call our approach data-driven material design. This combination of ML and synthesis is entirely original and, to our knowledge, has never been used in materials chemistry in the context of substrates for electrocatalytic reactions. Using an innovative “lab-in-the-loop” approach, we can effectively design advanced materials for electrocatalysis.

Scientific effect of the project: 1. Gaining scientific credibility through Open Science. 2. Encouraging the community to new technological solutions supported by digitization. 3. Improving methods or data for electrocatalysis. 4. Create new ML-based models that combine material structure and synthetic strategy with the electrocatalytic performance of porous nanocomposites (data-driven materials design). 5. Creation of new models that will show the correlation between structural parameters of substrates and electrocatalytic performance.