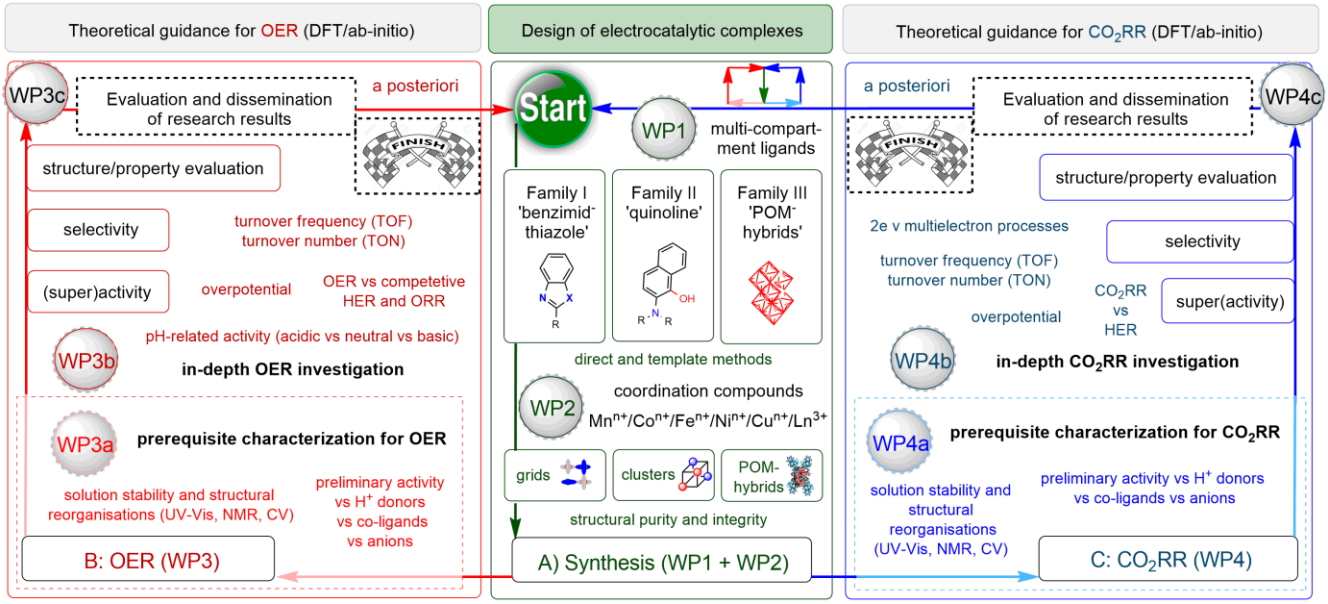
## Aim of the project

With a rising global population, impending climate change and increasing energy demands, major concerns have been raised over the security of our energy future. Developing sustainable, fossil-free pathways to produce fuels and chemicals of global importance should play a major role in reducing carbon dioxide emissions while providing the feed-stocks needed to make the products we use on a daily basis. One prospective goal is to develop electrochemical conversion processes that can convert molecules from the atmosphere ($H_2O$, $CO_2$) into higher-value products (e.g., hydrogen, hydrocarbons, oxygenates). Electrocatalysts play a key role in these energy conversion technologies, however they are still inadequate for practical applications. Therefore in the project we propose to synthesize a series of homo- and hetero- multimetallic coordination compounds with potential to improve the crucial electrocatalytic parameters such as increase the rate, efficiency, and selectivity of the chemical transformations of $CO_2$ and $H_2O$ small molecules.

## Concept and work plan

The work plan can be divided into four Work Packages **(WPs)** – **each representing specific objective** – which are gathered in three structured sections **A-C**. Our project will operate according to a stepwise approach between the different sections with the goal of the synthesis of electrocatalytic complexes that will expand the knowledge in the domains of OER and $CO_2$RR processes. Section **A** (green) covers ligand/complexes synthetic parts, Section **B** (red) focuses on studies related to OER, whereas Section **C** (blue) covers the $CO_2$RR related investigation.




Please note that we introduce the concept of the "**ongoing design of new compounds**", that proceeds through the three-level functionalization method. We start from the *a priori* design of the target molecule **TM1** on the grounds of literature survey, theoretical calculations and/or existing data. Upon successful synthesis (**A:** WP1+WP2), we proceed to the prerequisite WPs from sections **B** (WP3a) and **C** (WP4a) to determine if **TM1** exhibits the appropriate properties/features necessary for the in-depth investigation (OER – WP3b; $CO_2$RR – WP3b). This approach saves time and resources, but simultaneously increases our understanding of the structural design to ensure envisioned properties. Specifically, we can determine what hinders the positive outcome, and therefore *a posteriori* design of new target molecule **TM2** that is devoid of the drawbacks of **TM1** can be achieved. These will be ensured by theoretical guidance (DFT, *ab initio*, semiempirical methods) that are related to each electrocatalytic workpackage (OER – WP3c; $CO_2$RR – WP4c), with the ultimate goal of demonstrating the ***application of new complexes in electrocatalytic transformations of carbon dioxide and water.***

## Anticipated results

The proper selection, design and functionalization of *d*-/*f*-block complexes will lead to compounds, which will exhibit enhancement effects during electrochemical processes of inert reactants of importance to the electrochemical energy conversion and generation of fuels and utility chemicals. As such, a multifunctional character of the planned architectures will be demonstrated and eventually they will contribute to solving some of the global challenges, **which are in line with the European Green Deal policies and agendas presented during 2022 Davos World Economic Forum.**