Many of the commodities we use in our daily lives, such as materials, food or medicines, are obtained through processes that utilize catalysts. These catalysts enable the transformation of simple raw chemicals into molecules such as pharmaceuticals or agrochemicals. This process involves the making and breaking of chemical bonds, which typically requires a significant energy input. Thus, catalysts play a crucial role by weakening specific chemicals bonds and facilitating their formation under milder conditions. While most catalysts used are synthetic, nature also provides naturally occurring catalysts known as enzymes. Enzymes, as well as antibodies, provide reference points for selectivity and reactivity, but they are generally unsuited to industrial processes. In addition, enzymes exhibit remarkable specificity, generally catalyzing the conversion of only one type (or at most a few similar types) of substrate molecules into products. Understanding their reaction mechanisms has, however, been important in addressing the problem of how to achieve similar selectivity and reactivity in synthetic catalysts suited to industrial usage. Enzyme mechanisms typically involve substrate binding within a cavity formed by the protein superstructure, and a simple model of such a binding site is provided by molecules with defined cavity: capsules or cages.

Based on our years of experience and achievements, we propose to use the basics of coordination chemistry in the presented project to create a new generation of artificial enzymes based on water-soluble metallosupramolecular cages with interesting physicochemical properties. This is possible through the appropriate design of a series of ambident organic ligands with terminally located pyridine units, responsible for the formation of metallosupramolecular cages with Pd^{2+} ions, and chelating groups in the middle part, allowing for the introduction of appropriate functionalization (tuneable solubility, photoactivity) through the coordination of transition metal ions (Pd^{2+}, Co^{3+}, Ru^{3+}). The reaction between the ligands prepared in this way and the corresponding metal ions will represent a fundamental breakthrough in the generation of complex 3-dimensional systems, based in the first stage on the synthesis of suitable metalloligands with specific structure/properties tailored to individual needs, followed by the formation of the cage architecture. The characteristic lantern-type structure of the proposed cages imparts unique properties to the resulting structures: the almost spherical cavity shape is suitable for most guest molecules; the presence of acidic protons will support the formation of non-covalent interactions with said guests; and the cationic shell provides an ideal environment for anions. Therefore, another aspect of this project will be to investigate the separation/sequestration of halide anions from aqueous solutions. Defining the affinity for halides in the initial stage of the project will allow us to determine the (photo)catalytic potential in C-C and C-X bond transformation reactions.

The presented research project is eminently interdisciplinary in nature and covers many chemical fields, including organic chemistry, physical organic chemistry, and combinatorial chemistry, which have been identified under the common banner of supramolecular chemistry. The proposed idea of the project sheds light on a new direction for water-soluble metallosupramolecular systems, and the results obtained within the framework of the project will significantly contribute to the knowledge of designing functional cage systems with catalytic properties. The measurable effect of the project will be the development of 1) efficient and selective systems for the separation of anions from water, 2) efficient catalysts for substitution and coupling reactions in aqueous media.