Enzymes are proteins that act as biological catalysts by accelerating chemical reactions and are an indispensable part of every living organisms. Without enzymes almost no chemical reactions would be possible to perform.

The main idea behind this project is to study a relatively new group of complex chemical systems, that can act as artificial enzymes, catalyzing selected chemical reactions. These new systems, called polyoxometalates, have completely different structures from enzymes, but are biocompatible and were shown to be efficient catalysts. The specific goal of this project is to develop computational methods and models, based on quantum chemistry, that will allow to study their properties without the need of their synthesis (at least in the first stage of the studies). This will be both a time-effective and cost-effective approach that will allow to prescreen the candidates for artificial enzymes and select for further studies only those with the best predicted properties.

The proposed project will provide a tool for a rational design and study of various polyoxometalates and contribute to a better understanding of how to rationally design new classes of catalysts to serve specific purposes. It will also contribute to a better understanding of the structure-activity relationships for polyoxometalates, increase our knowledge about them, and, in the future, promise to create faster and more efficient catalysts. The proposed, comprehensive, theoretical approach to this problem will provide us with an accurate characterization of new systems and will lead to the development of a new methodology for the rational design of new catalysts and artificial enzymes. We believe that a project led by an expert in the theoretical description of catalytic systems is timely and relevant for the Polish catalysis landscape.