

Enzymes - proteins that catalyze chemical reactions - have fascinated researchers for years. They are fundamental to sustaining life, playing a crucial role in maintaining the processes that support living organisms.. Lastly, enzymes understanding and in consequence, the possibility of optimizing enzymes properties has been accelerated by the use of tools based on artificial intelligence and machine learning methods as well as high-throughput experimental methods pushing limits of performed analysis to millions per day. However, most of these methods have been dedicated to enzymes catalyzing reactions of molecules dissolved in solution, usually small ones. Meanwhile, enzymatic reactions occurring at the interface between two states of matter—liquid and solid—are still largely unexplored.

Among the exceptions, we can count enzymes that degrade natural polymers that build the world of plants, fungi and some animals: lignin, chitin and cellulose. Meanwhile, our industrial activities and the introduction of artificial, almost non-degradable polymers are forcing us to look for environmentally friendly solutions to reduce our adverse impact on the planet.

In our project, we want to look for methods to accelerate the design of enzymes capable of degrading complex heterogeneous synthetic polymers. We want to answer a number of questions: what factors regulate the specificity of enzyme binding to a solid, how selective this process can be, whether it is possible to take patterns from nature and teach enzymes to degrade plastics with often hydrophobic surfaces. For this purpose, we intend to develop computational and experimental methods and design enzymes that effectively degrade polyurethanes.