“Calculation of Electric Fields for Better Catalyst Design”

Chemical bonds are affected by electric fields, which are in turn sensitive to both short- and long-ranged molecular interactions. In this talk, I will show how we can therefore control chemical reactions by enabling a greater environmental organization of electric fields. More specifically, I will show that electric field calculations guided us to propose individual mutations for the de novo enzyme KE15 that contribute to the electrostatic stabilization of the transition state. Finally, I will illustrate the broader impact in catalysis of electric fields optimization by analyzing a supramolecular construct \((M_4L_6)\) that promotes the difficult reductive elimination from gold complexes.