"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.

SPECIAL SEMINAR

VALÉRIE VAISSIER WELBORN

UC-BERKELEY

Thursday, Jan. 10, 2019
3:30 pm in 1315 Chemistry

Coffee & cookies 3:15 pm