

DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE
SEMINAR SERIES
SPRING 2019

DATE: TUESDAY, MARCH 5
LOCATION: WEC Lecture Hall
TIME: 3:00PM-4:00PM

GUEST SPEAKER

Dr. Valerie Vaissier
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Department of Chemistry
University of California Berkeley
Berkeley, California

TOPIC

Calculation of electric fields for better catalyst design

ABSTRACT

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 (M4L6) that promotes the difficult reductive elimination from gold complexes.

BIO:

Valerie Welborn received an MSc (2010) and an advanced MSc (2011) in physics and chemistry from the Ecole Supérieure de Physique et Chimie Industrielle de la Ville de Paris (ESPCI), and received a MSc (2011) in theoretical and computational physics from Imperial College London. She received her PhD (2014) in Physics from the Doctoral Training Center in Theory and Simulation of Materials at Imperial College London (Physics department). She then spent two years as a postdoctoral researcher in the department of chemistry at Massachusetts Institute of Technology (MIT) where she worked with Troy Van Voorhis before joining the group of Teresa Head-Gordon at the University of California, Berkeley (Cal).

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