UCMERCED
UNIVERSITY OF CALIFORNIA
School of Natural Sciences

CHEMISTRY SEMINAR 291

Computational Chemistry Meets Photochemistry - Applications from Photobiology to Atmospheric Chemistry

Enrico Tapavicza
Department of Chemistry and Biochemistry
California State University, Long Beach

Date: 3/16/18
Time: 1:30 PM
Location: COB 267

For more information contact:
Christine Isborn
cisborn@ucmerced.edu

ABSTRACT

The recent theoretical developments of electronic structure methods for electronically excited states have opened the door for computational chemistry to study photochemical reactions. For instance time-dependent density functional theory (TDDFT) and more accurate approximate coupled cluster methods (CC2) allow to study excited states of large molecular systems. In this talk I will review theoretical developments to study the dynamics of excited state reactions. I will show how we use methods to unravel experimental findings in the photochemistry of vitamin D and atmospheric chemistry. A major focus is set on the simulation of ultrafast pump-probe experiments, and the the prediction of electronic spectra and product quantum yields. Besides gas phase photochemical reactions I will also discuss methods to include the chemical environment of a solvent.

BIO:

Enrico Tapavicza obtained his Ph.D. at EPFL in Switzerland in 2008 working on developing non-adiabatic molecular dynamics methods with Ursula Rothlisberger. He was a postdoctoral scholar in the group of Filipp Furche at the University of California Irvine before starting as a professor at CSU Long Beach in 2013.