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CHEMISTRY SEMINAR 291

Shining a Light on Photochemistry with Theoretical Chemistry

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Date: **4/6/18**
Time: **1:30 PM**
Location: **COB 267**

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ABSTRACT

My research group at California State University, Fullerton is broadly interested in studying processes related to photochemistry and non-adiabatic dynamics using the tools of theoretical chemistry. In the first part of my talk, I will focus on our efforts to achieve a mechanistic understanding of the intramolecular cyclization of oxime radical cations produced through photoinduced electron transfer. This collaborative project with Dr. Peter de Lijser at CSUF aims to not only determine the properties of reactive radical intermediates but also develop a new, green synthetic route towards complex heterocyclic molecules. In the second part of my talk, I will discuss our efforts to understand the internal conversion pathways through which kynurenine, a molecule found in the lens of our eyes, is able to rapidly and efficiently transform harmful ultraviolet light into heat. As part of this, I will describe our use of spin-flip time-dependent density functional theory to identify conical intersections between the S0 ground and S1 excited electronic states. I will end by giving an overview of a collaborative project with Nathan Kidwell at the College of William and Mary involving the non-adiabatic dynamics associated with the photodissociation of nitrophenol, a component of brown carbon aerosols.

BIO:

Professor Andrew Petit was a double major in Chemistry and Physics at the University of Pittsburgh, and received his Ph.D. degree in Chemical Physics with Professor Anne B. McCoy at the Ohio State University. He did his postdoctoral work with Professor Joseph E. Subotnik at the University of Pennsylvania. In 2016, he joined the faculty of California State University, Fullerton, and his research group uses theoretical and computational chemistry to model the spectroscopy and excited state dynamics of experimentally relevant systems.