



UCMERCED School of
UNIVERSITY OF CALIFORNIA Natural Sciences

CHEMISTRY SEMINAR 291

Electronic Dynamics in Complex Environments: From Electron Transfer to Singlet Fission

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Date: **4/20/18**

Time: **1:30 PM**

Location: **COB 267**

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ABSTRACT

Some of the most basic chemical reactions are those that involve primarily the motion of electrons with little rearrangement of the nuclei. Prominent examples include electron transport and excitonic energy transfer as well as more exotic phenomena such as singlet fission. These reactions are the centerpiece of artificial photosynthetic complexes, organic PVs and essentially all of redox chemistry. In treating the dynamics of these reactions, it becomes clear that knowledge of the molecular conformation alone is not sufficient to define a reaction coordinate (since the nuclei may not move appreciably during the course of the reaction). In this talk, we will discuss how the “reactant” and “product” states for these types reactions can be clearly defined using the electron density as the fundamental variable. We will then illustrate how this discovery has advanced our understanding of the building blocks of artificial photosynthesis: electron transfer in solution, energy transfer in films and singlet fission in organic photovoltaics.

