

CORE-CM SEMINAR
Michigan State University — Department of Chemistry

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Massachusetts Institute of Technology

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

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 illustrate the utility of this approach using two examples: electron transfer in solution and the simulation of singlet fission in organic photovoltaics.

Thursday, April 14, 2016

12:00 PM

Room 1400 – Biomedical and Physical Science Building

Professor Ben Levine - Host

Accommodations for persons with disabilities may be requested by calling the Chemistry Department at (517) 353-1083 two days prior to the event to ensure sufficient time to make arrangements. Requests received after this date will be met when possible.