CORE-CM SEMINAR
Michigan State University – Department of Chemistry and Department of Physics and Astronomy

Xiaosong Li
University of Washington
Department of Chemistry

Understanding Excitonic Dynamics using Time-Dependent Electronic Structure Theory

Excited state electronic dynamics are foundational to a wide range of chemical processes. For example, charge transfer and relaxation, crucial processes implicated in the function of photovoltaic and photocatalytic materials, are underpinned by time evolution of electronic degrees of freedom in response to external perturbations. The objective of the research in our group has been to develop time-dependent electronic structure methods designed to address some specific and important aspects of the dynamics of many-electron systems. The methods developed in our group have allowed us to explore new, interesting phenomena with the accuracy and detail needed to provide theoretical insights into results of cutting-edge experiments. In this talk, I will present several interesting case studies using our development of time-dependent electronic structure theory to understand photochemical dynamics of exciton and coherent multi-exciton with a focus on the generation, transfer, dephasing and polaron-assisted trapping. If time permits, I will also present our recent work on non-relativistic spin dynamics.

Thursday, Oct. 29, 2015
12:00 NOON
Room 1400 – Biomedical & Physical Sciences
Professor Rémi Beaulac – Host