University of Minnesota
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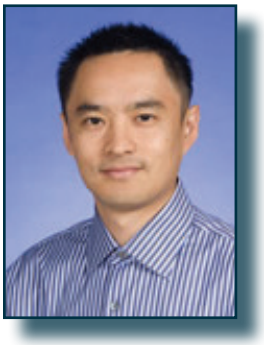
Department of Chemistry

Seminar

9:45 a.m. Thursday, October 23, 2014 • 331 Smith Hall



Asscoiate Professor

Xiaosong Li

Department of Chemistry
University of Washington

Time-Dependent Electronic Structure Theory: Excitonic, Charge-Transfer, and Spin Dynamics

Research focuses on the development of low-scaling methods to resolve excited state properties of many-electron systems, both in the time and frequency domains.

Website: http://depts.washington.edu/chem/people/faculty/li.html

Abstract

The time-dependent Schrodinger equation governs all non-equilibrium quantum mechanical processes of a many-electron system. These processes are crucial driving forces in many advanced scientific research and technological developments. For example, tuning the excitonic dynamics (i.e. excited many-electron dynamics) at bulk heterojunctions is an important step toward achieving high-quantum yield photovoltaics; the spontaneous magnetization (i.e., many-electron spin-dynamics) in diluted magnetic semiconductors determines their suitability for spintronic applications, etc. All of these phenomena are underpinned by many-electron dynamics which have transcendent impact on the photovoltaic and photocatalytic systems. In this talk, I will present the background of time-dependent many-electron theories and computational methods. I will also present recent applications of excited state electronic dynamics as exemplified by the excitonic dissociation dynamics in conjugated block copolymers and spin-dynamics of spin-frustrated systems.

Host: Jiali Gao
Refreshments will be served prior to the seminar.