CHEMISTRY & BIOCHEMISTRY

UCMERCED

DATE 09/12/2025 | TIME 01:30pm | LOCATION COB1 267

CHEMISTRY & BIOCHEMISTRY SEMINAR SERIES:

Quantum dynamics in molecular systems: Theory and application to photoinduced processes

Abstract:

The accurate theoretical treatment and simulation of dynamical processes in many-body quantum systems is a central goal in chemical and condensed matter physics. In this talk, I will discuss our recent work in this area. After an introduction to the topic and an overview of different dynamical methods, I will focus on time-dependent multiconfiguration methods. Formulated in the form of a tensor tree network, these variational basis-set methods facilitate the simulation of quantum dynamics in systems with many degrees of freedom.

Applications to photoinduced electron transfer processes are presented, including electron transfer in donor-acceptor complexes and electron injection at dye-semiconductor interfaces. Moreover, recent studies of singlet fission are discussed, a multiple exciton generation process in molecular materials. Focusing on intramolecular singlet fission, the mechanisms of this photophysical process are analyzed, in particular the role of the electronic states involved and the effect of electronic-vibrational coupling.

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About the Speaker:

Michael Thoss is a Professor of Physics at the University of Freiburg, Germany. He received his Diploma in Physics from the Ludwig Maximilian University of Munich in 1994 and his Ph.D. in Theoretical Chemistry from the Technical University of Munich in 1998. From 1998 to 2000, he was a Feodor-Lynen postdoctoral fellow of the Alexander von Humboldt-Foundation at the Department of Chemistry of the University of California at Berkeley. Afterwards he worked as a research associate and lecturer at the Department of Chemistry of the Technical University of Munich, where he finished his Habilitation in 2004. From 2009 to 2017 he was Associate Professor of Physics at the University of Erlangen, Germany.

His research focuses on the theory and simulation of dynamical processes in molecules and condensed matter. This includes the development of novel theoretical and computational methods as well as applications to investigate a variety of quantum dynamics and quantum transport processes. Recent examples comprise charge and energy transport processes in molecular nanostructures as well as photoinduced nonadiabatic reactions in molecules and at interfaces.

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