



CHEMISTRY & BIOCHEMISTRY SEMINAR SERIES:

Real-time simulations of non-equilibrium electron dynamics

Date:

9/29/2023

Time:

1:30 PM – 2:50 PM

Location:

COB1 267

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About The Speaker:

Joshua Kretchmer was born in San Jose, Costa Rica and grew up in Mill Valley, CA. He received his B.S. in Chemistry from UC Berkeley in 2009 and his Ph.D. as an NSF graduate research fellow from Caltech in December 2014 under the mentorship of Prof. Thomas Miller. He left Caltech for Princeton to join the group of Garnet Chan as a post-doctoral scholar. After the Chan group relocated to Caltech, he returned to finish his postdoc there. He joined the faculty of the Georgia Institute of Technology in 2019.



Abstract:

Non-equilibrium electron dynamics is prevalent throughout chemistry, biology, and physics, ranging from electron relaxation in ionized molecular clusters, to electron transfer in enzymatic systems, to charge transport in photoexcited materials. The direct simulation of electron dynamics presents a challenge for theoretical methods due to the time-dependent correlation between electrons. In this talk I will present two stories using real-time electronic structure methods to tackle this challenge. In the first, I will discuss our work using real-time DFT to simulate the ultrafast electronic decay mechanisms in weakly bound molecular systems. In the second, I will present our work developing a more sophisticated real-time quantum embedding method that allows for efficient simulations in extended systems.

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