



First Principles Dynamics for Photoactive Proteins

Prof. Todd Martinez



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12:30 p.m. - CiQUS Seminar Room

Prof. Todd Martinez
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<https://mtzweb.stanford.edu/>

Biosketch

- Postdoc, UCLA and Hebrew University, Jerusalem, Physical Chemistry (1996)
- PhD, UCLA, Physical Chemistry (1994)
- BS, Calvin College, Chemistry (1989)

Theoretical chemist Todd Martínez develops and applies new methods that predict and explain how atoms move in molecules. These methods are used both to design new molecules and to understand the behavior of those that already exist. His research group studies the response of molecules to light (photochemistry) and external force (mechanochemistry). Photochemistry is a critical part of human vision, single-molecule spectroscopy, harnessing solar energy (either to make fuels or electricity), and even organic synthesis. Mechanochemistry represents a novel scheme to promote unusual reactions and potentially to create self-healing materials that resist degradation. The underlying tools embody the full gamut of quantum mechanical effects governing molecules, from chemical bond breaking/formation to electron/proton transfer and electronic excited states.

Professor Martínez was born in Amityville, New York, but spent most of his childhood in Central America and the Caribbean. His chemical curiosity benefitted tremendously from the relaxed safety standards in Central American chemical supply houses, giving him unfettered access to strong acids and bases. When he also became interested in computation, limited or nonexistent computer access forced him to write and debug computer programs on paper. Today, Prof. Martínez combines these interests by working toward theoretical and computational modeling and design of molecules. Martínez received his PhD in chemistry from UCLA in 1994. After postdoctoral study at UCLA and the Hebrew University in Jerusalem, he joined the faculty at the University of Illinois in 1996. In 2009, he joined the faculty at Stanford, where

he is now the Ehrlam and Franklin Professor of Chemistry and Professor of Photon Science at SLAC National Accelerator Laboratory. He has received numerous awards for his contributions, including a MacArthur Fellowship (commonly known as the “genius award”). He is co-editor of Annual Reviews in Physical Chemistry, associate editor of The Journal of Chemical Physics, and an elected fellow of the American Academy of Arts and Sciences.

Current research in the Martínez lab aims to make molecular modeling both predictive and routine. New approaches to interactive molecular simulation are being developed, in which users interact with a virtual-reality based molecular modeling kit that fully understands quantum mechanics. New techniques to discover heretofore unknown chemical reactions are being developed and tested, exploiting the many efficient methods that the Martínez group has introduced for solving quantum mechanical problems quickly, using a combination of physical/chemical insights and commodity videogaming hardware.