UCMERCED | CHEMISTRY & BIOCHEMISTRY

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CHEMISTRY & BIOCHEMISTRY SEMINAR SERIES:

Discovering Chemistry and Photochemistry From First Principles Molecular Dynamics

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Abstract:

Novel computational architectures and methodologies are revolutionizing diverse areas ranging from video gaming to advertising and espionage. In this talk, I will discuss how these tools and ideas can be exploited in the context of theoretical and computational chemistry. I will show how the resulting advances in the efficiency of quantum chemistry can be harnessed to progress from traditional "hypothesis-driven" methods for using electronic structure and first principles molecular dynamics to a "discovery-driven" mode where the computer is tasked with discovering chemical reaction networks. We apply this reaction discovery method to methane pyrolysis, as an example where direct comparison to experimental results is possible. I show that the first principles method with no experimental input produces predictions in agreement with experiments and as good as bespoke models parameterized to experimental data. I then discuss the extension of these ideas to photochemical reactions involving electronic excited states. Finally, I describe our recent efforts to make computational chemistry tools broadly accessible for both education and research purposes.

About the Speaker:

Todd Martínez received his B. S. in Chemistry from Calvin College in 1989 and his Ph.D. in Chemistry from the University of California at Los Angeles in 1994. From 1994 to 1996, he was a Fulbright Junior Postdoctoral Researcher at Hebrew University in Jerusalem and a University of California President's Postdoctoral Fellow at UCLA. In 1996, he joined the faculty in the Department of Chemistry at the University of Illinois. He rose through the ranks to become the Gutgsell Chair in Chemistry. In 2009, he was recruited to join the faculty at Stanford University and the SLAC National Accelerator Laboratory, where he is currently David Mulvane Ehrsam and Edward Curtis Franklin Professor.

Professor Martínez' research lies in the area of theoretical chemistry, emphasizing the development and application of new methods which accurately and efficiently capture quantum mechanical effects of both electrons and nuclei. He pioneered the use of commodity videogame technology for computational chemistry and ab initio molecular dynamics. He has also developed new conceptual frameworks for understanding chemical reactivity induced by external force, i.e. "mechanochemistry."

Professor Martínez has received fellowships and/or awards from the Camille and Henry Dreyfus Foundation, the Alfred P. Sloan Foundation, the Arnold and Mabel Beckman Foundation, the David and Lucille Packard Foundation, and the John D. and Catherine T. MacArthur Foundation. Professor Martínez is an elected fellow of the American Physical Society, the American Association for the Advancement of Science, the American Academy of Arts and Sciences, the International Academy of Quantum Molecular Science and the National Academy of Sciences.

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