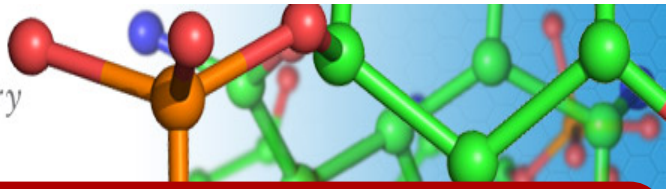
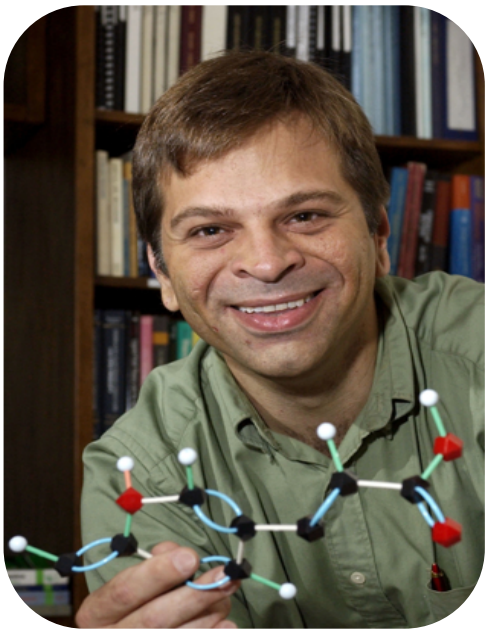
UNM | Department of Chemistry & Chemical Biology



Milton Kahn Annual Lectureship

Todd J. Martínez is a David Mulvane Ehrsam and Edward Curtis Franklin Professor of Chemistry at Stanford University and a Professor of Photon Science at the SLAC National Accelerator Laboratory. He received his B.S. from Calvin College in 1989 and his Ph.D. from UCLA in 1994. He was a Fulbright Fellow at the Fritz Haber Institute for Molecular Dynamics at Hebrew University and a University of California Presidential Postdoctoral Fellow at UCLA for two years prior to joining the faculty at the University of Illinois in 1996. He was named a Gutgsell Professor of Chemistry at the University of Illinois in 2006. He joined the Stanford faculty in 2009. Professor Martínez is a theoretical chemist whose research focuses primarily on developing first-principles approaches to chemical reaction dynamics, starting from the fundamental equations of quantum mechanics.

Friday, March 3rd, 2017
SMLC 102
4:00pm



Todd J. Martinez

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Discovering Chemistry with Advanced Computing and Machine Learning

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 discuss how insights gleaned from recommendation systems (such as those used by Netflix and Amazon) can lead to reduced scaling methods for electronic structure (solving the electronic Schrodinger equation to describe molecules) and how the algorithms in electronic structure can be adapted for commodity stream processing architectures such as graphical processing units. I will show how these advances 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. Finally, I will show how these can be combined with force-feedback (haptic) input devices and three-dimensional visualization to create molecular model kits that carry complete information about the underlying electrons. This interactive first principles molecular dynamics method (molecular computer-aided design or mCAD) opens the door to novel ways of teaching chemistry and may also be of use in applied chemical research.