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CHEMISTRY SEMINAR 291

Ab Initio Molecular Dynamics: New Methods and Fundamental Studies in Enzyme Reactions

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Date: 3/17/17
Time: 1:30 PM
Location: COB 267

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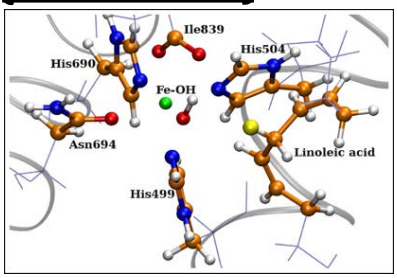
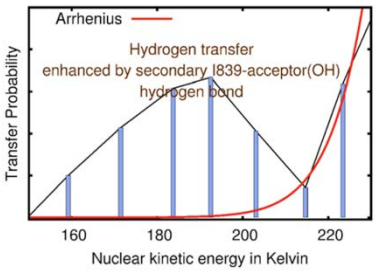
ABSTRACT





One part of this talk deals with new computational methods for the simultaneous dynamical treatment of electrons and nuclei, where the electrons are treated at extremely high quantum chemical (such as CCSD) accuracy. In the second part of the talk, we discuss our recent work on the rate-determining hydrogen transfer step in the catalytic transformation of fatty acids by the enzyme Soybean Lipoxygenase-1. This enzyme is a non-heme metalloprotein and the catalytic process shows the remarkably large H/D KIE of 81. While we have studied this in the past, this talk will focus on the "computational discovery" of a new hydrogen bond (between the Fe-OH hydrogen and Ile839 on the figure above) that modulates the hydrogen transfer (transferring hydrogen shown in yellow). We find that when this hydrogen bond is "turned off" in our computational experiments, the H-transfer stops. Furthermore, this hydrogen bond also leads to the non-Arrhenius behavior that we note on the figure to the right.

BIO:

Srinivasan Iyengar received an integrated M.Sc. Degree in Chemistry from the Indian Institute of Technology, Bombay, India; an M.S. in Chemistry from the University of Florida, Gainesville, FL; and a Ph.D. from the University of Houston, under the auspices of Professor Donald J. Kouri. He joined the Indiana University in Fall 2003 after assuming two post-doctoral positions, one under the direction of Professor Gustavo E. Scuseria at Rice University, Houston, TX and the second under the supervision of Professor Gregory A. Voth at the University of Utah. Research efforts in the Iyengar group are on the interface of chemistry, computational physics and applied mathematics. They deal with the development of new theoretical methods and the subsequent implementation of these into efficient computational models. The methods are derived with an aim to help solve problems in biophysical chemistry, atmospheric chemistry and the area of nano-material science. Specifically, current research efforts are directed towards the fundamental understanding of the interplay between electrons and nuclei. The areas of study include hydrogen-bonded systems, hydrogen transfer reactions, and the study of electron transport in molecular-wire-type systems. To study these problems we have developed several new computational methodologies.

Iyengar has been the recipient of the Arnold and Mabel Beckman Young Investigator Award (2006-2009), the Camille and Henry Dreyfus New Faculty award (2003-2008), and Shell and Dow Chemical awards as graduate student at University of Houston. At Indiana he has also been the recipient of the summer faculty fellowship.