TCI SEMINAR

# Quantum fluctuations in chemical systems: from atmospheric science to biology

## Monday, February 11, 2013
## 3:00 pm Room 8335


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Over the past decades molecular simulation has become an increasingly important tool in predicting and interpreting chemical processes. Inherent in these simulations is the assumption that the nuclei behave classically. However, for processes involving light particles such as hydrogen the quantum mechanical nature of the particles can dramatically alter their structure and dynamics. Recently we have developed highly efficient approaches to treat quantum mechanical fluctuations in condensed phase systems and to calculate isotope effects. These advances allow us to investigate, in unprecedented detail, chemical systems where the inclusion of quantum mechanical effects is essential to obtain the correct result. In this talk I will discuss these developments and illustrate their utility with recent applications ranging from the geochemically important fractionation of hydrogen isotopes between liquid water and its vapor to the biologically relevant proton delocalization in enzyme active sites. I will also discuss how simple harmonic approximations to the isotope effect in these systems can be both inefficient and misleading.


Theoretical Chemistry Institute Seminar Series