Physical Chemistry Seminar

Tuesday, October 19, 2010 | **11:00 a.m.** | **Room 1315 Chemistry Building**

Vibrational Overtone Induced Chemical Reactions in Gas and Cluster Phase

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Unimolecular chemical reactions of small organic molecules induced by vibrational overtone excitation are studied using theoretical simulations. It is found that the photochemical reactions often proceed by pathways far distant from the conventional intrinsic reaction coordinate. When the reaction occurs in hydrogen bonded water clusters, quantum chemistry calculations suggest that transition state barrier is often greatly lowered and thus one might expect significant acceleration of the rate through water catalysis. Simulations reveal, however, that the catalytic effect is often suppressed through competition with water evaporation. The validity of ab initio dynamics simulations that employ classical mechanics is assessed using a large scale wave packet simulation of the six-dimensional HOOH→2OH problem.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students and Post Docs may meet with the speaker at 1:00 p.m. in Room 8335