

Physical Chemistry Seminar

Tuesday,
October 9, 2012

11:00 am

Room 1315
Chemistry Building

Atomistic Simulations of Spectroscopy and Reactive Processes in the Gas- and Condensed Phase



Professor Markus Meuwly

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Host: Professor Qiang Cui

I will discuss computational methods applied to current problems in the gas- and condensed phase. Particular emphasis will be on atomistic simulations with validated force fields and how they affect the quality of the simulations in comparing with experimental data. This, combined with methods to follow reactions in the gas- and condensed phase, provides access to a multitude of valuable information because phase space can be extensively sampled. Processes considered include the vibrational spectroscopy of IR-probes in proteins, energy transfer between solute and solvent, and dissociation dynamics of sulfuric acid in the gas phase. It will be discussed how a combination of experiment and atomistic simulations can lead to a deeper understanding of common physico-chemical processes at an atomistic level.

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

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