# ”Structure and Ultrafast Vibrational Dynamics of Strongly Hydrogen-Bonded Complexes”

## PHYSICAL SEMINAR

**Monday, November 23rd, 2015**
**4:00 p.m.**
**Hutchison Hall 473**
**University of Rochester**
**Department of Chemistry**


Guest Speaker: Professor Poul B. Petersen
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Chemistry and Chemical Biology



**Abstract:** Hydrogen-bonded structures are ubiquitous in biological systems, where they provide stability and can act as proton transfer relays. Medium and strongly hydrogen-bonded structures often exhibit very broad and complex vibrational structures that challenges both experiments and theoretical modeling alike. Here we present ultrafast pump-probe and 2D-IR spectroscopy of medium and strongly hydrogen-bonded dimers as well as DFT calculations modeling the broad vibrational spectra. The calculations show that the driving force for the width of the vibrational structures is low frequency modes that modulate the hydrogen-bonding strength of the high-frequency OH/NH modes spreading them over several hundred wavenumbers. This in turn brings the OH/NH modes into contact with Fermi-resonances with bending modes causing the vibrational substructure. The ultrafast vibrational experiments utilize a continuum mid-IR probe pulse spanning the entire vibrational range. The pump-probe experiments examine the vibrational energy relaxation pathways and show that the NO/NH modes to not relax to the vibrational hot ground state within a few hundred femtoseconds, as previously suggested. The 2D-IR experiments reveal strong vibrational couplings both among the high-frequency modes and between the high and fingerprint modes of these complex systems.



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