CFEL SCIENCE

SEMINAR

24th June 2011, 2:30 - 3:30 p.m.
HASYLAB Bld. 25f / Seminar Room 456

Yoshitaka Tanimura
Department of Chemistry Kyoto University

Calculating and Analyzing Multidimensional Spectroscopies from the reduced hierarchy equations of motion approach

Spectral line shapes in a condensed phase contain information from various dynamic processes that modulate the transition energy. In this talk, we explore and describe the roles of different physical phenomena that arise from the peculiarities of the system-bath coupling in multidimensional spectra. For this purpose, we employed the Brownian oscillator model with the nonlinear system-bath interaction. Using the hierarchy formalism, we could precisely calculate multidimensional spectra for a single and multimode anharmonic system for inter- and intramolecular vibrational modes. We examined the capability of the present approach by comparing the signals of two- and three-dimensional IR vibrational spectroscopy obtained from experiments and molecular dynamics simulations. A role of quantum dissipative dynamics is also examined by comparing classically and quantum mechanically calculated multidimensional spectra.

REFERENCES:

Y. Tanimura and A. Ishizaki, Acc. Chem. Res. 42, 1270 (2009).
http://pubs.acs.org/doi/abs/10.1021/ar9000444

Y. Tanimura: J. Phys. Soc. Jpn. 75 (2006) 082001.
http://jpsj.ipap.jp/link?JPSJ/75/082001/

Host: R. J. Dwayne Miller, CFEL