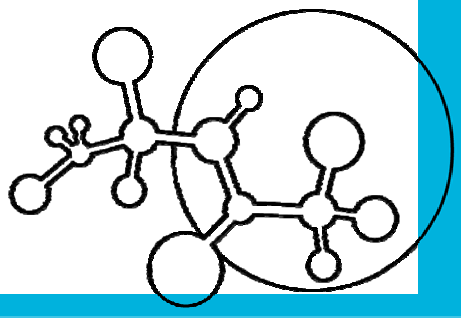
FRIAS
FREIBURG INSTITUTE FOR ADVANCED STUDIES
ALBERT -LUDWIGS -UNIVERSITÄT FREIBURG
SCHOOL OF SOFT MATTER RESEARCH



Quantum Efficiency Seminar and Colloquium

Maja Kobus

Institute of Physics,
Albert Ludwigs-Universität Freiburg

Dynamics and spectroscopy of peptide vibrations

Proteins and peptides are chains composed of characteristic peptide groups (-C-C=O-N-H-), that form beta-sheet or helical structures. Since the C=O stretch vibrations of the peptide backbone, this band is highly sensitive to the structure and dynamics of the system, time-resolved infrared (IR-) experiments of these modes have been employed to monitor structural motion on several time scales. The method has also been used to track the energy transport along the backbone. Applying two-dimensional (2D)-IR spectroscopy, moreover, the homogeneous and inhomogeneous relaxation times are distinguishable. Due to the complexity of these spectra, experiments need theoretical support. Our approach to model the vibrational properties of peptides is based on a quantum-classical description. It consists of a classical all-atom molecular dynamics simulation of the structures of the system combined with density functional theory calculations of the conformation-dependent solvent- and peptide-induced frequency fluctuations. The vibrational Hamiltonian is formulated in an exciton-like manner [1]. Within this approach we study the various time scales of the frequency fluctuations, which directly report on the peptide dynamics at various temperatures [2]. Solving the Schrödinger equation allows us to study excitonic transfer features of the vibrational energy along the peptide backbone, including the study of spatial coherence effects [3]. In order to make connection to experiments, the 2D-IR signals are simulated, allowing us to interpret the signal features in terms of dynamical structure and environment changes.

[1] Nonadiabatic vibrational dynamics and spectroscopy of peptides: A quantum-classical description, M. Kobus, R. D. Gorbunov, P.H. Nguyen, and G. Stock, Chem. Phys. 347, 208 (2008)

[2] Infrared signatures of the peptide dynamical transition: A molecular dynamics simulation study, M. Kobus, P.H. Nguyen, and G. Stock, J. Chem. Phys. 133, 034512 (2010)

[3] Coherent vibrational energy transfer along a peptide helix, M. Kobus, P.H. Nguyen, and G. Stock, J. Chem. Phys. , submitted

Date: **Tuesday, February 8th, 2011 2:15 pm**

Location: **FRIAS Seminar Room, Albertstr. 19, Freiburg**

Contact: Andreas Buchleitner, Institute of Physics, Quantum Optics and Statistics,
T +49 761 203 5929 F +49 761 203 5967 E beate.spingler@frias.uni-freiburg.de
www.physik.uni-freiburg.de

Physikalisches Institut
Albert-Ludwigs-
Universität Freiburg