MO 26: Poster: Biomolecules

Time: Thursday 16:00–18:00 Location: P2

MO 26.1 Thu 16:00 P2

Isomerization dynamics of conformer-selected molecules — •Melanie Schnell — Max-Planck-Advanced Study Group at the Center for Free-Electron Laser Science, D-22607 Hamburg — Max-Planck-Institut für Kernphysik, D-69117 Heidelberg

Isomerization reactions are a fundamental class of chemical transformations that are omnipresent in many areas of molecular science. Many molecules, such as amino acids or small sugars, exhibit multiple structural isomers, which are distinct species with individual physical and chemical properties. A detailed understanding of their isomerization dynamics will help us to gain better insight into important processes in chemistry and biology, such as molecular recognition.

Novel broadband rotational spectroscopy allows for recording spectra with widths of up to 11 GHz in a single measurement. This opens the door to new directions of rotational spectroscopy, such as dynamic rotational spectroscopy - a novel way to study conformational isomerizations of highly vibrationally excited complex molecules on the picosecond time scale. We are currently setting up a new experiment based on conformer selection using an electrostatic deflector and on broadband rotational spectroscopy to investigate the isomerizations of small sugars, amino acids and their complexes with picosecond resolution. On the poster, I will present this new technique and report on the present status of the experiment, its prospects and challenges.

MO 26.2 Thu 16:00 P2

Spectroscopy on Single RC-LH1 Complexes of the Photosynthetic Purple Bacterium *Rhodopseudomonas acidophila* — •Paul Böhm[1], June Southall[2], Richard Cogdell[2], and Jürgen Köhler[1] — [1]Experimental Physics IV, University of Bayreuth, 95440 Bayreuth, Germany — [2]Institute of Molecular, Cell & Systems Biology, College of Medical, Veterinary and Life Sciences, University of Glasgow, Glasgow G12 8QQ, Scotland

The reaction center (RC) light-harvesting 1 (LH1) complexes form a basic building block in the photosynthetic apparatus of purple bacteria, where each LH1 complex directly surrounds a RC. In the course of the photosynthetic process a quinol molecule has to leave the RC and pass through the LH1 complex to be further converted by other protein complexes. There is an ongoing discussion in literature whether LH1 complexes include a gap in their structure, thus enabling quinol transport, or if LH1 complexes completely surround the RCs.

To date no structural details are known for the RC-LH1 complex of *Rhodopseudomonas (Rps.) acidophila* investigated in this work. By comparing spectral characteristics of single-molecule spectra from RC-LH1 complexes of *Rps. acidophila* with those of RC-LH1 complexes with a better known structure, we gained new insights into the unknown LH1-structure from *Rps. acidophila*. Since spectral features found for RC-LH1 complexes of *Rps. acidophila* resemble those of open LH1 complexes, we propose that the LH1 complex of *Rps. acidophila* also has a gap in its structure, rather than being completely closed.

MO 26.3 Thu 16:00 P2

Plasmonic Enhancement of Light Harvesting Complex-Fluorescence — •Sebastian R. Beyer[1], Simon Ullrich[2], Stefan Kudera[2], Richard J. Cogdell[3], and Jürgen Köhler[1] — [1]Experimental Physics IV and Bayreuther Institut für Makromolekülforschung (BIMF), University of Bayreuth, 95440 Bayreuth, Germany — [2]Max-Planck-Institute for Metals Research, Dept. of New Materials and Biosystems, 70569 Stuttgart, Germany — [3]Institute of Molecular, Cell and Systems Biology, College of Medical, Veterinary and Life Sciences, Biomedical Research Building, Glasgow G12 8QQ, Scotland, UK

We present the first evidence of plasmon induced fluorescence enhancement on Pigment-Protein-Complexes from Purple Bacteria. Using fluorescence microscopy, we recorded fluorescence intensities of single Light Harvesting Complex 2 molecules (LH2) from *Rhodobacter sphaeroides* in the presence of an ordered array of gold nano spheres. Evaluating the fluorescence intensities of more than 13000 single LH2, we found mean fluorescence enhancement up to factor 2.5 with the strongest single event reaching factor 13.7.

MO 26.4 Thu 16:00 P2

Fluorescence excitation spectroscopy of individual chlorosomes of *Chlorobium Tepidum* — •Marc Jendrny[1], Thijs J. Aartsma[2], and Jürgen Köhler[1] — [1]Experimental Physics IV, University of Bayreuth, 95448 Bayreuth, Germany — [2]Department of Biophysics, University of Leiden, 9504 RA Leiden, The Netherlands

Chlorosomes are the main light-harvesting antennae complexes in green photosynthetic bacteria. These complexes feature a rod-like shape of 100 nm - 200 nm length and 20 nm - 50 nm width and consist of thousands of bacteriochlorophyll *c*, *d* or *e* depending on the species. The major difference from other light harvesting complexes is that the chromophores are not embedded into a protein-scaffold. It is assumed that these antenna complexes show a large variation with respect to size and that the mutual arrangement of the chromophores features a helical component giving rise to strong circular dichroism. We measured polarization-resolved fluorescence-excitation spectra from individual Chlorosomes of the green sulfur bacterium Chlorobium Tepidum this uncovers that the well known ensemble absorption band in the spectral range from 720 nm - 770 nm has contributions from at least two electronic transitions.

MO 26.5 Thu 16:00 P2

Combining an Ion Mobility Spectrometer with IR spectroscopy — •Stephan Warnke, Gerard Meijer, and Gert von Helden — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The shape and three-dimensional structure of large molecules or clusters in the gas phase is of interest but difficult to investigate. While in the condensed phase various structure-resolving methods exist, methods applicable to gas phase molecules are limited. Two structure-sensitive methods are IR spectroscopy and ion mobility spectrometry (IMS). In IMS, molecules are ionized and they subsequently drift through a buffer gas under the influence of an electric field. Species with different collisional cross sections are separated after many collisions with the buffer gas molecules. By measuring the drift time of each species, information about its structure can be obtained. The combination of IMS with IR spectroscopy therefore yields complementary information as IR spectroscopy is sensitive to the local environment while IMS is more sensitive to the global structure.

We are in the process of building a machine consisting of a nano-ESI source and a drift cell (i.e. the IMS part) prior to a quadrupole mass spectrometer and an ion trap with optical access for spectroscopy on conformer and mass/charge selected ions. The design of the ion mobility spectrometer and first experimental results will be presented.

MO 26.6 Thu 16:00 P2

2D spectra of excitonic systems with large reorganisation energy — •Birgit Hein[1], Christoph Kreisbeck[1], Tobias Kramer[1], and Mirta Rodriguez Pinilla[2] — [1]Institute for Theoretical Physics, University of Regensburg, Germany. — [2]Instituto de Estructura de la Materia, Madrid, Spain.

We present the results of a GPU computation of 2D-echo spectra of the Fenna-Matthews- Olson complex, a part of the light harvesting complex of green sulphur bacteria. This complex has a coupling between the exciton and vibrational states and experiments show long-lived quantum beatings which have been observed at 77K (Engel, et al. (2007), Nature, 446, 782) and 294 K (Collini, et al. (2010). Nature, 463 644). This beatings cannot be reproduced with a Markovian approach. In 2009 Ishizaki and Fleming introduced an hierarchical but numerically very demanding algorithm to simulate such systems. We tackle the computationally effort by calculating the 2D-echo spectra on graphic processing units (GPU).

MO 26.7 Thu 16:00 P2

GPU implementation of hierarchical equations for energy transfer in light harvesting complexes — •Christoph Kreisbeck[1], Mirta Rodriguez Pinilla[2], Birgit Hein[1], and Tobias Kramer[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Instituto de Estructura de la Materia, Madrid, Spain

Recent experiments (Engel *et al.* Nature 2007, Collini *et al.* Nature 2010) show evidence for quantum coherences in light harvesting complexes, which prevail up to physiological temperatures. These finding suggest that coherence might enhance efficiency of energy transfer to the reaction center of photosynthese systems. Besides wave like motion, to achieve high efficient energy transfer, coupling to the vibrational environment plays an important role. This coupling is rather large and non-perturbative as well as non-Markovian approaches are required. The most accurate approach is provided by the hierarchical equations (HE) proposed by Ishizaki and Fleming in 2009. The HE require considerable memory and computational efforts. To overcome the numerical limitations we implement the HE on a high performance graphics processing unit (GPU). This allows us to study the transfer efficiency over a wide range of parameter such as reorganization energy or temperature. The efficient GPU implementation yields enormous speedups and the computation times are close to those of Markovian approaches. This facilitates to fit future experiments instead of Markovian theories to the more accurate HE. References see www.quantumdynamics.de

MO 26.8 Thu 16:00 P2

Raman Spectroscopy — A Rapid Tool for Food Investigation

— •Rasha Hassanein, Patrice Donfack, Pinkie Eravuchira, Bernd von der Kammer, and Arnulf Materny — Center of Functional Materials and Nanomolecular Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Raman scattering gives access to the vibrational fingerprints of molecules. Recently, Raman spectroscopy has been introduced in food analysis since it can provide content-relevant information based on well-defined and resolved spectra in various sample categories. The major advantages of this technique lies in the fact that it requires no or only little sample preparation, it is a rapid and nondestructive tool, and when combined with a fiber-optic sampling station, can make such a system ideally suited for in-line industrial processing. In our research, we have demonstrated the capabilities of dispersive Raman spectroscopy using visible excitation in combination with appropriate chemometric methods for the investigation of different food types, such as edible oils, citrus oils, milk, and green coffee. The advantage of using an excitation with visible light (VIS) is the increased signal intensity in general and in some cases (*e.g.* for carotenoids) the resonance enhancement, which helps to detect also constituents at lower concentrations. In our contribution, we will present the potential of Raman spectroscopy with VIS excitation for the investigation various food types.