# MO 26: Poster: Biomolecules

Time: Thursday 16:00–18:30 Location: Lichthof

MO 26.1 Th 16:00 Lichthof

**Spectroscopic Investigation of Reaction-Center Light-Harvesting 1 Complexes from *Rhodopseudomonas acidophila* - Influences of the Environment** — •Paul Böhm[1], Ralf Kunz[1], Tobias Pflock[1], June Southall[2], Richard Cogdell[2], and Jürgen Köhler[1] — [1]Experimental Physics IV and Bayreuth Institute of Macromolecular Research (BIMF), University of Bayreuth — [2]Division of Biochemistry and Molecular Biology, Institute of Biomedical and Life Sciences, University of Glasgow

Reaction-center (RC) light-harvesting 1 (LH1) complexes from *Rhodopseudomonas (Rps.) acidophila* were studied in 3 different environments. At first the applicability of the two types of detergents N,N-Dimethyldodecylamnin-N-oxide (LDAO) and *n*-Dodecyl *β*-D-maltoside (DDM) for the stabilization of the RC-LH1 complexes was tested. And finally the complexes were also reconstituted into lipid vesicles.

Comparing room-temperature absorption spectra of LDAO- and DDM-stabilized complexes we discerned a slight redshift of 1 nm for the characteristic B875-band in the DDM environment. This redshift which also occured for the reconstituted sample and a better temporal stability of the RC-LH1 complexes in DDM solution, indicate that this detergent is a good mimicry of the natural environment. Low-temperature (1.4 K) fluorescence-excitation and emission spectra of bulk ensembles both showed distinct redshifts (6.6 nm and 8.4 nm), when comparing the detergent-stabilized and the reconstituted samples, reflecting a great structural flexibility for these complexes.

MO 26.2 Th 16:00 Lichthof

**Probing Molecular Profiles of Tumorigenicity in Colon Carcinoma Differential Tumor Cells Associated with a Tumor-Specific Lipid Marker by Raman Spectroscopy** — •Patrice Donfack[1], Gabriele Multhoff[2], and Arnulf Materny[1] — [1]Jacobs University Bremen, Germany — [2]Klinikum rechts der Isar, TU München, Germany

Studying detailed differentiation steps of tumorigenicity is a rather challenging task, which leads towards the understanding of the molecular details of tumorigenicity. We present Raman spectroscopic studies of differential tumorigenic CX- and CX+ cells, in combination with multivariate analysis. These cells are sublines of human colon carcinoma cell lines, with differential Hsp70 membrane expression pattern associated with a tumor-specific lipid component. Raman spectroscopy has revealed protein-dominated spectra of CX- and CX+ with slight differences in the lower wavenumber region. However, changes in the protein bands around 2933 $cm^{-1}$, where prominent lipid bands are expected, are more dramatic. These observations support the assumption that tumorspecific lipid markers interact with key proteins that play an important role in tumor progression such as cell growth regulation. Changes in the cell's lipid composition lead to changes in important protein components. Changes observed for CX- and CX+ have been subjected to multivariate analysis for resolving the Raman signatures of tumorigenicity from the bands at 1094, 1300, 1450, 1656, and about 2933 $cm^{-1}$. Further insights can be gained by surface enhanced Raman scattering of the CX-/CX+ pecific lipid globoyltriaosylceramide Gb3.

MO 26.3 Th 16:00 Lichthof

**Discrimination between Arabica and Robusta Green Coffee Using Visible Raman Spectroscopy and Chemometric Analysis** — •Rasha Hassanein, Patrice Donfack, and Arnulf Materny — Jacobs University Bremen, Bremen, Germany

Raman spectroscopy is a rapid and nondestructive method, which gives information about the chemical composition of a sample without the necessity for special sample preparation. Therefore, it is ideally suited for online industrial monitoring processing. In this contribution, we will present our newest work, where we have successfully demonstrated the application of VIS Raman spectroscopy in combination with principal component analysis (PCA) as a rapid technique for the discrimination between the two coffees species, Arabica and Robusta without any extraction. Raman spectra of Arabica and Robusta revealed prominent contributions from their chlorogenic acid (CGA) and lipid content. Starting with the complete Raman spectra in the range from 500 to 3050 $cm^{-1}$, the spectral range between 1000 and 1750 $cm^{-1}$ has proven statistically significant for the distinction between the two coffee species. This part of the spectrum is dominated by the Raman bands of CGA and based on the PCA scores 93% of the spectral variation was explained by the first two principal components (PCs), suggesting that CGAs account for the most important spectral variation in the complete spectral range. Nonetheless, restricting the analysis uniquely to the spectral range from 2700 to 3050 $cm^{-1}$ which contains the lipid Raman bands a reliable discrimination of Arabica and Robusta coffee was also achieved.

MO 26.4 Th 16:00 Lichthof

**Fluorescence Blinking of the RC-LH1 core complex from** *Rhodopseudomonas palustris* — Sarah Unterkofler[1], •Tobias Pflock[1], Richard Cogdell[2], and Jürgen Köhler[1] — [1]Experimentalphysik IV, Universität Bayreuth, D-95447 Bayreuth — [2]Glasgow Biomedical Research Centre, University of Glasgow, UK

We present low-temperature (1.5 K) fluorescence blinking studies on individual RC-LH1 core complexes of the photosynthetic bacterium *Rhodopseudomonas palustris*.

For the majority of the recorded time traces, blinking could not be observed within the experimental time resolution. For the complexes where blinking could be resolved, the „off-times“ as well as „on-times“ were power-law distributed. These times are associated with the charge-separated state of the reaction centre (RC). We discuss the findings in the context of blinking experiments that have been performed on quantum dots [1] as well as on molecular systems [2].

[1]R. Verberk et al., Phys. Rev. B 66, 233202 (2002)
[2]D. Ernst et al., Chem. Phys. Lett. 482, 93 (2009)

MO 26.5 Th 16:00 Lichthof

**Zwei-Photonen-Anregungspektroskopie des Lichtsammelkomplexes LHC II** — Alexander Betke[1], Bernd Voigt[1], Heiko Lokstein[2] und •Ralf Menzel[1] — [1]Institut für Physik und Astronomie, Universität Potsdam — [2]Institut für Biochemie und Biologie, Universität Potsdam

Xanthophylle sind wesentliche Komponenten von photosynthetischen Pigment-Protein-Komplexen höherer Pflanzen. Im Wechselspiel mit Chlorophyll dienen sie je nach Lichtverhältnissen der Effizienzsteigerung des Lichteinfangs oder der Photoprotektion, u.a. der nichtphotochemischen Dissipation überschüssiger Anregungsenergie. Am Anregungsenergietransfer zwischen den Pigmenten sind auch deren niedrigste Singulett-Anregungszustände ($S_1$) beteiligt. Die Untersuchung des Xanthophyll-$S_1$-Zustands wird dadurch erschwert, dass dieser für Einphotonen-Übergänge vom Grundzustand symmetriebedingt verboten ist. Jedoch können diese „dunklen“ Zustände mittels simultaner Zweiphotonen-Absorption selektiv erreicht werden. *In vivo* gibt der so bevölkerte Xanthophyll-$S_1$-Zustand seine Energie ultraschnell an den energetisch nahen Chlorophyll *a* $Q_y$-Zustand weiter und wird über Chlorophyll-Fluoreszenz detektierbar. *In vitro* hingegen kann der Xanthophyll-$S_1$-Zustand charakterisiert werden, indem nach der Zweiphotonen-Anregung transiente Absorption gemessen wird. Es werden neue Ergebnisse vergleichender Messungen an der Lichtsammelantenne LHC II diskutiert, die mit unterschiedlichen Xanthophyllen komplementiert wurde. Dieser Beitrag wird von der DFG im Rahmen des SFB 429/TP A2 gefördert.

MO 26.6 Th 16:00 Lichthof

**Determination of Milk Fat Unsaturation Degree Using Raman Spectroscopy** — •Pinkie J Eravuchira, Rasha Hassanein, Patrice Donfack, Bernd von der Kammer, and Arnulf Materny — Jacobs University Bremen, Germany

The knowledge of the composition of milk fat is of paramount importance both for the desired quality and the shelf-life of the final milk product. Specifically, the unsaturation level of milk is a good indication of its healthiness, where a higher unsaturation level also means a less stable product. A rapid in-line detection technique would be an ultimate development that would help the manufacturer to estimate the milk fat unsaturation level and consequently decide about additives in order to increase the shelf life of the final milk product. Traditional methods for determining the unsaturation level of milk fat require tedious chemical analyses. Raman spectroscopy is already being successfully applied for food quality control. Raman spectra of fat

show characteristic fingerprints at 1265, 1300 and 1654 $cm^{-1}$ that are directly connected with the unsaturation degree in the carbonic chain of fat molecules. In our contribution, we apply Raman spectroscopy in combination with chemometric analysis as a rapid tool for the quantification of milk fat unsaturation level, and we compared our results with the standard "iodine value" detection method and find a good agreement. We therefore evaluate the potential of the Raman technique for the milk fat unsaturation level detection directly without the need for separating the fat from the milk, an aspect that would be convenient for in-line monitoring.

MO 26.7 Th 16:00 Lichthof

**Absorption spectra of molecular aggregates at finite temperature** — •Sebastian Möbius[1], Gerhard Ritschel[1], Jan Roden[2], Alexander Eisfeld[2], and Walter Strunz[1] — [1]Institut für Theoretische Physik, Dresden, Germany — [2]MPIPKS, Dresden, Germany

We compare different methods to calculate molecular absorption spectra for a monomer in a thermal environment. Starting with a master equation that describes the molecular system and a finite temperature bath, it is possible to derive an expression for the absorption spectrum using the quantum regression theorem. On the other hand, approaches via stochastic Schrödinger equations are discussed: first, the influence of a thermal environment can be replaced by a suitably chosen Markov process. Secondly, employing colored processes, the dynamics of the vibrational degrees of freedom at finite temperature may be described efficiently by c-numbers as well [1]. Aiming at absorption spectra of molecular aggregates, we investigate the efficiency of stochastic methods.

[1] J. Roden, A. Eisfeld, W. Wolff, W. T. Strunz, Phys. Rev. Lett. 103, 058301 (2009)

MO 26.8 Th 16:00 Lichthof

**Energy transport in small molecular aggregates at finite temperature** — •Gerhard Ritschel[1], Sebastian Möbius[1], Jan Roden[2], Alexander Eisfeld[2], and Walter T. Strunz[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

We present an efficient stochastic Schrödinger equation method to treat molecular aggregates with a single relevant vibrational degree of freedom for each monomer in a thermal environment. Based on ideas developed for non-Markovian open quantum systems, the vibrational degrees of freedom and the thermal bath may be replaced by colored stochastic processes such that the ensuing Schrödinger equation propagates states of the electronic degrees of freedom only [1]. The method is applied to study optical properties and energy transport in aggregates of coupled monomers at finite temperature.

[1] J. Roden, A. Eisfeld, W. Wolff, W. T. Strunz, Phys. Rev. Lett. 103, 058301 (2009)