BP 8: Posters: Protein Structure & Dynamics

Time: Monday 17:15–20:00 Location: P3

BP 8.1 Mon 17:15 P3

Conformational Adsorption Reaction of BSA on the Surfaces of Nanosilica and Nanodiamond — •Victor Wei-Keh Wu — Department of Chemical and Materials Engineering, National Kaohsiung University of Applied Sciences(KUAS), 80782 Kaohsiung City, Taiwan — Victor Basic Research Laboratory e. V.(VBR) Gadderbaumer-Str. 22, D-33602 Bielefeld, Germany

From the fluorescences (excitation at 280 nm) of BSA of 0-10000 nM in 7 mM PPBS at pH=4.70 before and after adsorption reactions on the surfaces of nanosilica(NS) and nanodiamond(ND) of diameter 100 nm as suspension solutions($50\mu g/20\mu L$), the adsorption thresholds, reaction constants as well as coverages have been obtained. Adsorption thresholds were located at 150 nM for both systems. The adsorbed BSA were 420 mg for two partices in g; 28.0 and 7.64 mg, on unit surface in m^2 of NS and ND, respectively. Adsorption constants $1.2x10^8$ and $3.7x10^7$ $(nM)^{-1}$ for systems BSA+NS and BSA+ND, respectively, have been obtained. Comparing with the respective constants $1.2x10^7$ and $6.5x10^7$ for systems lysozyme+NS and lysozyme+ND, the biomolecular conformations as well as behaviors are different. The spatial fitting between depression or hole on the nanosurface as carrier, and dimension of the protein with significant activity should also be considered, besides the charge-charge interactions between the surface and protein, and among the proteins. Financial aids by groups 510 and NB11 of IAMS, Taipei, and VBR, Bielefeld; support with Fluorescence Spectrophotometer F-4500 FL, Hitachi, Japan, by KUAS are acknowledged. **Ref.** V. W.-K. Wu and F. Kure, *Chin. J. Chem.* **28**(2010).

BP 8.2 Mon 17:15 P3

L-edge X-Ray Spectroscopy Revealing Structure and Dynamics of Metalloprotein Active Centers — •Kathrin Maria Lange[1], Ronny Golnak[1], Sebastien Bonhommeau[2], and Emad Flear Aziz[1,3] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Str. 15, 12489 Berlin — [2]Institut des Sciences Moléculaires, UMR 5255 CNRS, 351 cours de la Libération, 33405 Talence Cedex, France — [3]Freie Universität Berlin, FB Physik, Arnimallee 14, D-14195 Berlin, Germany

Reactions catalyzed by metalloproteins occur at their active centre, accordingly determining its electronic structure allows drawing conclusions about the protein function. We revealed for the first time the electronic structure of metalloproteins in physiological media using L-edge X-ray absorption spectroscopy on the iron active centre.1 By comparing the electronic structure of haemoglobin and catalase, the origin of the high enzymatic activity of catalase could be revealed.2 Furthermore the preferential ligation of myoglobin was investigated recently.3 The electronic structure of its iron active centre upon binding to O2, CO, CN and NO were compared to the reduced form and metmyoglobin. For the interpretation of the data muliplet calculations were used.

1 E F Aziz et al., Phys. Rev. Let. 102, 68103 (2009)

2 N Bergmann et al., Phys. Chem. Chem. Phys. Vol. 12, 18, 4827-4832 (2010)

3 K M Lange et al., in preparation (2010)

BP 8.3 Mon 17:15 P3

Effect of thermostating and electrostatics on the wildtype LOV1 domain of phototropin and its mutants — •Emanuel Peter, Bernhard Dick, and Stephan A. Baeurle — Fakultät für Chemie und Pharmazie, Universität Regensburg, 93040 Regensburg, Deutschland

Phototropins are blue-light photoreceptors in plants and algae, which consist of 2 LOV-(light oxygen voltage sensitive)-domains and 1 kinase domain. Each LOV-domain contains a noncovalently bound flavin-mononucleotide-(FMN)-chromophore, which after absorption of blue light at around 450 nm undergoes a photoreaction with a cysteine-residue attached to an apoprotein, inducing a signal in the organism via the kinase-domain. Both the signal transduction as well as the mechanism of the photoreaction of these domains are still only poorly understood. In this presentation we show results of molecular dynamics simulations, where we investigated the effect of electrostatics and thermostating on the solution structure and dynamics of signal transduction of the LOV1-domain. We compare the calculation results with various experimental data and demonstrate that these computational issues have an important influence on the equilibrium and time behavior of such systems.

BP 8.4 Mon 17:15 P3

Anomalous diffusion of oligomerized transmembrane proteins — •Ulrich Schmidt[1,2] and Matthias Weiss[1,3] — [1]Cellular Biophysics Group, German Cancer Research Center, c/o BIOQUANT, Im Neuenheimer Feld 267, 69120 Heidelberg — [2]Laboratory for Computational Cell Biology, Department of Cell Biology, Harvard Medical School, Boston, USA — [3]Experimental Physics I, University of Bayreuth, 95440 Bayreuth

Transmembrane proteins frequently form (transient) oligomers on biomembranes, e.g. while participating in protein sorting and signaling events. Using coarse-grained membrane simulations we show here that transmembrane proteins show a subdiffusive motion on short time scales when being part of a linear oligomer, i.e. a flexible polymer, embedded in a two-dimensional membrane. Our results are in agreement with previous experimental observations. They further indicate that polymers of transmembrane proteins are well described by predictions from Rouse theory in two dimensions even in the presence of hydrodynamic interactions

BP 8.5 Mon 17:15 P3

Rigidity analysis of HIV-1 protease — Jack Heal, Stephen Wells, Emilio Jimenez-Roldan, and •Rudolf Roemer — Department of Physics and Centre for Scientific Computing, University of Warwick, Coventry, CV4 7AL, United Kingdom

We show the effect of different inhibitors on the rigidity profile of HIV-1 protease as it unfolds. A rigidity analysis of 40 protein crystal structures from the protein data bank is made using the software FIRST. The results are compared with and without inhibitors present. This study builds on a recent comparative study of protein structures using FIRST. In a simulated rigidity dilution, the unfolding pattern of the protein can be observed. The presence of an inhibitor slows the rigidity loss, in particular around the active site of the enzyme. FIRST is not computationally demanding and its results can be calculated on a timescale of CPU-minutes. We study protein mobility along low-frequency normal modes of motion using the FRODA software and the elastic network model. The presence of an inhibitor changes the extent to which the protein is able to move in these directions.

BP 8.6 Mon 17:15 P3

Investigation of self-assembled desmin filament networks by atomic force microscopy — •Mareike Dieding[1], Volker Walhorn[1], Andreas Brodehl[2], Hendrik Milting[2], and Dario Anselmetti[1] — [1]Experimentelle Biophysik und Angewandte Nanowissenschaften, Fakultaet für Physik, Universitaet Bielefeld, Universitaetsstr. 25, D-33615 Bielefeld — [2]Herz- & Diabeteszentrum NRW, E. & H. Klessmann-Institut fuer Kardiovaskulaere Forschung und Entwicklung, Georgstr. 11, D-32545 Bad Oeynhausen

Arrythmogenic right ventricular cardiomyopathy (ARVC) is an inherited heart muscle disease, frequently accompanied by sudden cardiac death and terminal heart failure.

Various point mutations of the intermediate filament desmin are potential candidates for the trigger factor [1]. Desmin serves as a mechanical integrator of neighboring Z-discs in the sarcomere and also as an important structural component of the intercalated disc by binding to desmosomal plaque proteins.

We investigated the self-assembled desmin network structure by means of atomic force microscopy (AFM) under ambient conditions in topographic experiments. We were able to reveal various mutation specific structural defects in the desmin network. Our *in vitro* results are supporting additional *in vivo* confocal laser scanning microscopy (CLSM) studies of desmin-transfected cells.

[1] B. Klauke et al., De novo desmin-mutation N116S is associated with arrhythmogenic right ventricular cardiomyopathy, Hum. Mol. Genet. 19 (23), 2010

BP 8.7 Mon 17:15 P3

Winkelabhängige Ramanspektroskopie an Photosystem-II-Kristallen — •Georg Bens[1], Katharina Brose[1], Athina Zouni[2]

und Janina Maultzsch[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Institut für Chemie, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany

Das Photosystem II ist als Ort der Wasseraufspaltung ein elementarer Bestandteil der Photosynthese. Im Reaktionszentrum des Photosystems II befinden sich drei β-Carotinmoleküle, deren Funktion bisher ungeklärt ist. Es wurde vorhergesagt, dass das Carotin CarD2 aus dem Reaktionszentrum am Elektronentransport nach der Wasserspaltung beteiligt ist [1] . Begründet wird dies durch das Vorhandensein eines Carotinkations im belichteten Reaktionszentrum. Da die Carotinmoleküle im Reaktionszentrum unterschiedliche Orientierungen aufweisen, versuchen wir mittels polarisationsabhängiger, resonanter Ramanspektroskopie und der winkelabhängigenen Signalcharakteristik zu bestimmen, welches der verschieden orientierten Carotinmoleküle ionisiert wird. Da das Carotinkation eine andere Resonanzfrequenz und ein anderes Ramanspektrum als neutrales β-Carotin hat, kann man es gut von den anderen Carotinmolekülen des Photosystems unterscheiden. Auf diese Weise soll identifi*ziert werden, welches der Carotine ionisiert wird.

[1] Schenderlein, M.: Elektronentransferprozesse in den Photosystemen I & II, Dissertation TU Berlin, 2010
http://opus.kobv.de/tuberlin/volltexte/2010/2586/

BP 8.8 Mon 17:15 P3

Tip-Enhanced Raman Spectroscopy on Membrane Proteins — •Elmar Hassan Hubrich, Kenichi Ataka, and Joachim Heberle — Free University of Berlin, Department of Physics, Exp. Molecular Biophysics, Arnimallee 14, 14195 Berlin, Germany

Tip-enhanced Raman spectroscopy (TERS) combines high spatial resolution of atomic force microscopy (AFM) with structural sensitivity of surface-enhanced Raman spectroscopy (SERS). Using a gold-coated AFM tip, it is possible to measure Raman signals with high spatial resolution ($\sim$30 nm).

The AFM allows imaging, measuring (e.g.: single-molecule force microscopy), and manipulating matter at the nanoscale. The information is gathered by "feeling" the surface with a mechanical probe.

Raman spectroscopy provides information about the molecular structure of proteins. In order to detect monolayer we use surface-enhanced Raman spectroscopy (SERS). The SERS signal is enhanced in the vicinity of (usually) silver- or gold-coated surfaces (up to a factor of 10^{9-12} compared to conventional Raman).

Up to now, this novel technique is mainly applied to surfaces modified with inorganic samples. However, TERS is a promising tool in investigation of membrane proteins since single molecules could be studied at atomic level by Raman spectroscopy under native biological conditions.

Here, we introduce the experimental setup and discuss the application of TERS to the investigation of membrane proteins.

BP 8.9 Mon 17:15 P3

Molecular docking study of histone deacetylases 1 and 3 in interaction with the benzamide histone deacetylase inhibitor MS-275 — •Davoud Pouladsaz[1], Azadeh Ebrahimi[2], and Michael Schreiber[1] — [1]Institut für Physik, Technische Universität Chemnitz — [2]Institut für Hirnforschung, Eberhard Karls Universität Tübingen

Numerous studies have shown that abnormal HDAC activity is associated with oncogenesis. On the other hand, HDAC inhibition has been reported in several studies to induce tumor cell differentiation, apoptosis, and cell cycle arrest. In this scheme, HDACs are considered potential targets for cancer therapy. One of the novel HDAC inhibitors is MS-275, a benzamide derivative with *in vivo* antitumor activity and selectivity against HDAC1 and HDAC3. However, the precise molecular and cellular mechanisms by which MS-275 acts to modulate HDAC activity have yet to be determined. In this work, we use molecular docking techniques to identify the active sites of HDAC1 and HDAC3 in interaction with MS-275. The results provide template structures for further drug experiments.