BP 17: Posters: Protein structure and dynamics

Time: Monday 17:30–19:30   Location: Poster A

BP 17.1   Mon 17:30   Poster A

mFES: A robust molecular Finite Element Solver for electrostatic energy computations — ●Ernst-Walter Knapp and Ilkay Sakally — Institut für Chemie und Biochemie, Freie Universität Berlin

We present a robust method for the calculation of electrostatic potentials of large molecular systems using tetrahedral finite elements (FE). Compared to the finite difference (FD) method using a regular simple cubic grid to solve the Poisson equation, the FE method can reach high accuracy and efficiency using an adaptive grid. Here, the grid points can be adjusted and are placed directly on the molecular surfaces to faithfully model surfaces and volumes. The grid point density decreases rapidly toward the asymptotic boundary to reach very large distances with just a few more grid points. A broad set of tools are applied to make the grid more regular and thus provide a more stable linear equation system, while reducing the number of grid points without compromising accuracy. The latter reduces the number of unknowns significantly and yields shorter solver execution times. The accuracy is further enhanced by using second order polynomials as shape functions. Generating the adaptive grid for a molecular system is expensive, but it pays off, if the same molecular geometry is used several times as is the case for pKA and redox potential computations of many charge variable groups in proteins. Application of the mFES method is also advantageous, if the molecular system is too large to reach sufficient accuracy when computing the electrostatic potential with conventional FD methods.

BP 17.2   Mon 17:30   Poster A

Transmembrane-peptide structure formation from coarse-grained simulations — ●Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Interfacial systems are at the core of fascinating phenomena in many disciplines, such as biochemistry, soft-matter physics, and food science. However, the parametrization of accurate, reliable, and consistent coarse-grained (CG) models for systems at interfaces remains a challenging endeavor. I will describe recent advancements made toward the description of secondary-structure formation of peptides in a membrane environment using CG models. By combining a lipid model that can semi-quantitatively reproduce material properties of a fluid membrane bilayer and a peptide model that is not biased toward one particular state (e.g., α-helix or β-sheet), the combined parametrization allows to look at how peptide structure is affected by the membrane environment on long timescales. I will illustrate the robustness of the model by looking at different WALP transmembrane helical peptides starting from stretched, unstructured conformations. Analysis of the structure of the membrane during folding provides insight into the local deformation during helix formation as a function of chain length (16 to 23 residues). Finally, the method is used to fold the 50-residue-long major pVIII coat protein (fd coat) of the filamentous fd bacteriophage. The results show excellent agreement with experimental structures and atomistic simulations in implicit membrane, demonstrating that such a protocol can serve as a starting point for better-refined atomistic simulations in a multiscale framework.

BP 17.3   Mon 17:30   Poster A

Variation of Exciton-Vibrational Coupling in Photosystem II Core Complexes from Thermosynechococcus elongatus as Revealed by Single-Molecule Spectroscopy — ●Sepideh Sknadary[1], Martin Hussels[1], Thomas Renger[2], Frank Müh[2], Athina zouni[3], Alfred Meixner[1], and Marc Brecht[1,4] — [1]Universität Tübingen, IPTC and Lisa + Center, Tübingen, Germany — [2]Johannes Kepler Universität, Institut für Theoretische Physik, Linz, Austria — [3]Humboldt-Universität zu Berlin, Berlin, Germany. — [4]Zurich University of Applied Science Winterthur (ZHAW), Winterthur, Switzerland

Photosystem II (PSII) is the membrane protein complex of higher plants, green algae and cyanobacteria that uses solar energy to catalyze the electron transfer from water to plastoquinone. The PSII core complex (PSIIcc) is composed of the two intrinsic antenna protein subunits; CP43 and CP47, coordinating 13 chlorophyll a (Chl) a and 16 Chls, respectively, the D1D2cyt b-559 reaction center complex, that coordinates 6 Chl a and 2 pheophytin a molecules, and several additional small subunits. The spectral properties and dynamics of the fluorescence emission of PSIIcc are investigated by single-molecule spectroscopy (SMS) at 1.6 K. The emission spectra are dominated by sharp zero-phonon lines (ZPLs), which are the result of weak to intermediate exciton-vibrational coupling and slow spectral diffusion. Overall results show that electrostatic, rather than exchange or dispersive interactions are the main contributors to the exciton-vibrational coupling in this system.

BP 17.4   Mon 17:30   Poster A

Solvation of 2GB1 in ionic liquid/water mixtures — ●Volker Lesch[1], Vasileios A. Tatsis[1], Andreas Heuer[1], Christian Holm[2], and Jens Smiatek[2] — [1]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster — [2]Institut für Computerphysik, Universität Stuttgart

Ionic liquids are considered as environmentally friendly compared to organic compounds. Furthermore, they have an ionic character which leads to interesting solvation properties.

We present molecular dynamics simulations of the protein 2GB1 in explicit water and doped with the ionic liquid 1-ethyl-3-methylimidazolium acetate (4.55 mol/l). The solvation of the protein as well as the solvent's structure induced from the protein were investigated on the atomistic scale. The protein is stabilized by the ionic liquid because of specific interactions.

BP 17.5   Mon 17:30   Poster A

Dimensionality reduction of protein dynamics by employing distance and contact analysis — ●Matthias Ernst and Gerhard Stock — University of Freiburg, 79104 Freiburg, Germany

To describe and understand protein dynamics, a reduction of the 3N-6 dimensional space of the N atoms involved is crucial. A commonly employed way to reduce dimensionality is principal component analysis (PCA), a linear transformation which removes linear correlations of the coordinates by diagonalizing their covariance matrix. As PCA results depends strongly on the type of coordinates, use of internal coordinates like dihedral angles (dPCA[1]) instead of cartesian atomic coordinates often provides higher resolution, especially for large-amplitude motion e.g. found in folding systems[2]. In contrast to dihedral angles which mainly reflect the behaviour of neighbouring residues in a protein, distances between pairs of atoms also contain information about residues further apart in the primary sequence.

We employ and classify different types of PCA for dimension reduction by quantities based on information theory and on their structural resolution. We show that analysis based on contact distances support the findings gained by dPCA and facilitate interpretation and visualization of the folding process by highlighting which contacts contribute to the folding transitions.

[1] Y. Mu, P. H. Nguyen, and G. Stock, Proteins **2005**, *58*, 45.
[2] F. Sittel, A. Jain and G. Stock, J. Chem. Phys. **2014**, *141*, 014111.

BP 17.6   Mon 17:30   Poster A

Insoluble proteins in presence of salt: a computational study — ●Patrick Kreissl and Jens Smiatek — Institut für Computerphysik, Universität Stuttgart, 70569 Stuttgart, Germany

Nogo-60 is a truncated sixty residue version of the extracellular domain of the human Nogo proteins. It is soluble in pure water but highly insoluble in buffer. Surprisingly, the protein almost completely consists of three large α-helices. However, the last six residues remain highly unstructured. If this six residue tail is dropped, another protein—Nogo-54—is designed, which is soluble in both buffer and pure water. Nogo-60 and Nogo-54 thus provide an almost identical primary structure but different solubility/insolubility properties.

Both proteins were simulated in different salt solutions as well as in pure water to get an idea of the underlying mechanisms and to study the influence of the salt ions on the protein solvation behavior.

BP 17.7   Mon 17:30   Poster A

Multivalent interaction of hemagglutinin with sialic acid as studied by scanning force microscopy and force spectroscopy — ●Valentin Reiter[1], Manuel Gensler[1], Sumati Bhatia[2], Luis Cuellar[2], Daniel Lauster[3], Rainer Haag[2], An-

dreas Herrmann[2], and Jürgen P. Rabe[1] — [1]Department of Physics, Humboldt-Universität zu Berlin — [2]Institute of Chemistry & Biochemistry, Freie Universität Berlin — [3]Department of Biology, Humboldt-Universität zu Berlin

The glycoprotein hemagglutinin (HA) is a transmembrane protein of the influenza virus that comprises over 80% of the envelope proteins present in the virus particle and accounts for the primary attachment of the virion to a target cell. The attachment happens due to hydrogen bonds between the three binding pockets of the HA globular domain and sialic acid (SA) molecules on the biological cell surface. The development of efficient inhibitors of virus binding requires precise knowledge of this interaction. On protein immobilizing surfaces the scanning force microscope (SFM) can be used to directly probe the bond strength of single and multiple HA - SA - interactions. SFM images are used to determine the surface density of the immobilized proteins. Then, single molecule force spectroscopy with cantilevers functionalized with SA is employed to measure the rupture forces between HA-SA bonds. The dissociation behavior is calculated from the distribution of rupture forces at various pulling speeds.

BP 17.8   Mon 17:30   Poster A
Local water dynamics around antifreeze protein residues in the presence of osmolytes: The importance of hydroxyl and disaccharide groups — •anand narayanan krishnamoorthy[1], jens smiatek[2], and christian holm[3] — [1]Institute for Computational Physics,University of Stuttgart — [2]Institute for Computational Physics,University of Stuttgart — [3]Institute for Computational Physics,University of Stuttgart

It is nowadays common knowledge that the antifreeze activity of AFPs is mainly determined by a short -range effect which includes a direct binding in the ice phase. Recently, experimental findings also revealed a long range effect which implies a significant retardation of the water dynamics to facilitate the ice binding process specifically for AFGPs. The aim of the work is to examine the dynamics of water molecules around different antifreeze protein residues by using atomistic molecular dynamics simulations. The analysis of the water hydrogen bond characteristics and the dipolar relaxation times reveals a strong retardation effect of water dynamics around the AFGP prototype. Our numerical results reveal the significant importance of polar units like threonine and dissacharides for the direct binding of water molecules in terms of hydrogen bonds and a significant retardation of water dynamics. In addition, our findings indicate that this effect is even more pronounced in the presence of kosmotropic osmolytes.

BP 17.9   Mon 17:30   Poster A
Electric field induced secondary structure changes in small peptides — •Sina Zendehroud, Bernhard Reuter, and Martin E. Garcia — Theoretical Physics, University of Kassel, Kassel, Germany

The conformation of a protein is pivotal for its physiological functionality. Hence procedures to manipulate secondary and tertiary structure formation, including the use of external electric fields, are of great interest. Referring to predictions based on previous calculations that applied a reduced model and the Monte Carlo method [P. Ojeda-May and M. E. Garcia, Biophys. J. **99**(2), 595-599 (2010)], we investigated if they hold true making use of a more complex all-atom model. Using the molecular dynamics package GROMACS and the CHARMM force-field, we performed all-atom simulations of a small peptide under the influence of external static electric fields. We observed that the electric field modifies the secondary structure of the peptide and can even induce a transition from beta-sheet to alpha-helix or helix-like structures.

BP 17.10   Mon 17:30   Poster A
Apolipoprotein A1 adsorption at solid/liquid and liquid/air-interfaces — •Susanne Dogan[1], Irena Kiesel[1,2], Matthias Kampmann[1,3,4], Kolja Mende[1], Florian J. Wirkert[1], Michael Paulus[1], Christian Sternemann[1], and Tolan Metin[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]Institut Laue-Langevin, 38000 Grenoble, France — [3]DESY, D-22603 Hamburg, Germany — [4]Department of Physics, University of Siegen, D-57072 Siegen, Germany

One of the most important high density lipoproteins for the lipid metabolism is apolipoprotein A1 (ApoA1), which has a ring-like structure. The inner part of the ring is hydrophobic whereas the outer part is hydrophilic. Due to this, ApoA1 forms structures with lipids and cholesterol. In order to study the adsorption behavior of ApoA1, x-ray reflectivity experiments at the hydrophobic solid/liquid interface were performed at beamline BL9 of the synchrotron light source DELTA (Dortmund, Germany). The measurements were conducted at different temperatures (25°C-80°C). To investigate the adsorption of ApoA1 at negatively charged surfaces, a DPPA monolayer at the liquid/air-interface at room temperature was used. The results indicate an adsorption and deformation with a conformational transition of the tilted ring of ApoA1 over several non-separated states with increasing temperature at hydrophobic interfaces. No significant change in the profile of DPPA was observed when the DPPA film was prepared on ApoA1 solutions. Thus, the electrostatic repulsion between ApoA1 and the head groups of DPPA prevents the adsorption at the membrane.

BP 17.11   Mon 17:30   Poster A
Water Dynamics Near Fluorinated Amino Acids: A Molecular Dynamics Study — •João R. Robalo and Ana Vila Verde — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Incorporating fluorinated amino acids into proteins often results in increases of protein resistance to thermal and chemical degradation, as well as in improved functionality. Recent work by B. Koksch and co-workers [1] suggests that changes in protein function upon fluorination of amino acids at the protein active site may arise from the different behavior of water near those amino acids, compared to their non-fluorinated analogues. At present, however, the structure and dynamics of water near fluorinated proteins is not understood. We are addressing this issue by developing classical, all-atom, fixed-charge models of fluorinated hydrophobic amino acids and using them to investigate water structure and dynamics in their vicinity. The models are parameterized to reproduce experimental free energies of hydration of fluorinated analogues of hydrophobic amino acid side chains. The developed models shall then be used for the study of water near fluorinated small peptides and proteins.

[1] - B. Koksch, unpublished

BP 17.12   Mon 17:30   Poster A
Investigating interactions of anions with selectins using molecular dynamics simulations — •Sadra Kashef Ol Gheta and Ana Vila Verde — Max Planck Institute of Colloids and Interfaces

Selectins are well known for their role in the adhesion of leukocytes and platelets to the endothelium that takes place, e.g., during inflammation. Because of the important biological role played by selectins, much effort has been put into finding artificial ligands that effectively compete with the natural ones. Recently, dendrimeric polyglycerol (dPG) polymers functionalized with various anionic functional groups were investigated for their potential as L-selectin inhibitors. It was found that the affinity of dendrimers for selectin depends strongly on the nature of the anionic group, increasing in the order carboxylate < phosphate < phosphonate, sulfonate < bisphosphonate <<< sulfate. To understand the molecular origin of this anionic series, we use classical all-atom models based on the CHARMM36 force field for proteins and explicit water to characterize the intrinsic interactions between various anionic functional groups and positively charged amino acids using small molecule analogues, e.g., methylsulfate, methylamine. The results from classical simulations are compared against those from ab initio calculations, to assess the quality of the classical models.

BP 17.13   Mon 17:30   Poster A
Langevin Modeling of Biomolecular Dynamics — •Björn Bastian and Gerhard Stock — University of Freiburg, 79104 Freiburg, Germany

Total simulation times long enough to capture biologically relevant functions are often inaccessible by Molecular Dynamics (MD) simulations on the level of full atom Newton equations. The data driven Langevin equation (dLE) technique allows for efficient propagation of a few selected system coordinates up to long simulation times on the basis of many short continuous MD trajectories (that can be computed in parallel) [1]. Beforehand, important system coordinates to describe conformational dynamics are obtained by dimensionality reduction, e.g. by principal component analysis.

If the timescales of slow system and fast bath variables separate, a general nonlinear Langevin equation can be derived from a microscopic Hamiltonian by projection techniques. The dLE algorithm presented obtains the drift, friction and diffusion fields by a local estimation on MD data. Thus dLE trajectories yield a correct global energy land-

scape without the requirement of input data being correctly Boltzmann weighted. Here, we present an algorithm that can treat full second-order Langevin equations in several dimensions due to more stable estimators. As proof of principle, we demonstrate the recovery of the stochastic fields for a test model.

[1] Schaudinnus N, Rzepiela AJ, Hegger R, Stock G. Data driven Langevin modeling of biomolecular dynamics. J. Chem. Phys. 138, 204106 (2013).

BP 17.14   Mon 17:30   Poster A
Biomolecules at gold-water interfaces: the role of the metal polarization — •Isidro Lorenzo[1], Hadi RAmezani-Dakhel[2], Hendrik Heinz[2], and Marialore Sulpizi[1] — [1]Johannes Gutenberg University Mainz, Staudinger Weg 7 55099 Mainz — [2]Departament of Polymer Engineering, University of Akron, Ohio 44325

Microscopic understanding and control of protein-surface interactions is gaining an increasing interest due to the new development of bio-interfaces for medical and bio-technological applications. In this contribution we aim to provide a characterization of different peptides / gold interactions at a molecular level in order to explain and interpret recent surface experimental results [1]. We have devised a novel scheme to include the metal polarization (image charge effect) induced by the adsorbed molecules into atomistic simulations. Our scheme can easily complement currently used 12-6 Lennard-Jones potentials [2], as included in simulation packages as GROMACS and LAMMPS. Extensive tests have been performed for the force field validation and comparisons with quantum mechanics (QM) density functional theory (DFT) calculations are also discussed. Results for aminoacids and nucleic acids nano assembly different gold surfaces are presented.

[1] V. Humblot, A. Tejeda, J. Landousi, A. Vallee, A. Naitabdi, A. Taleb, C.-M. Pradier. Surface Science 2014, 628, 24-29.
[2] Heinz H, Vaia RA, Farmer BL, Naik RR J. Phys. Chem. C 2008, 112, 17281 17290; Heinz H, Farmer BL, Pandey RB, Slocik JM, Patnaik SS, Pachter R, Naik RR. J. Am. Chem. Soc. 2009, 131, 9704-9714

BP 17.15   Mon 17:30   Poster A
Studying *in situ* protein adsorption and bacterial adhesion via fast scanning AFM and force spectroscopy — •Christian Spengler[1], Nicolas Thewes[1], Thomas Faidt[1], Christian Kreis[2], and Karin Jacobs[1] — [1]Saarland University, Experimental Physics, 66041 Saarbrücken, Germany — [2]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

Protein adsorption and bacterial adhesion are the first steps in biofilm formation. Hereby, proteins serve as a conditioning layer for the further attachment of bacteria and other organisms. Hence, the understanding and control of protein layers and their interaction with bacteria is an important task relevant to life sciences and engineering. We study the protein adsorption in situ on a single protein level. For this purpose, we use a fast scanning AFM operating in liquid under flow conditions which reveals single protein adsorption events. The surfaces for these experiments are hydrophilic and hydrophobized silicon substrates with different oxide layer thickness and very smooth artificial tooth samples. Additionally, we characterize the bactericidal activity of proteins in their adsorbed state using purified peptidoglycan. Furthermore, we perform single cell force spectroscopy to investigate the adhesion of bacteria to these protein layers in comparison to the bare surface.

BP 17.16   Mon 17:30   Poster A
Protein Folding: Driving forces and external influences — •Bernhard Reuter, Pedro A. Ojeda May, and Martin E. Garcia — University of Kassel, Theoretical Physics II, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

One of the most important questions of nature sciences is why a given amino acid sequence under physiological conditions mostly exists in a certain functional spatial structure - the native state. If certain proteins misfold in bigger amounts it results in serious health impairments like neurodegenerative diseases (i.e. Alzheimer's and prion diseases). In this context the question of the effect of external influences on the stability of the native state arises. To address this problem the effect of an external electric field on the peptide V3-loop 1NJ0 was analyzed by Monte Carlo simulations. It was revealed that a strong electric field induced a transition from a beta-sheet into a helix conformation. Also the effect of an spatial temperature gradient on a proteinlike designed heteropolymer was simulated using the Langevin Dynamics method showing that a temperature gradient can facilitate protein folding.

BP 17.17   Mon 17:30   Poster A
Selective Adsorption of Similar-Sized Proteins into a Nanoporous Silica Glass — •Sebastian T Moerz[1,2] and Patrick Huber[1,2] — [1]Experimental Physics, Saarland University, D-66041 Saarbruecken — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, D-21073 Hamburg

The adsorption of lysozyme, cytochrome c and myoglobin, similar-sized globular proteins of approximately 1.5 nm radius, into the mesoporous silica material SBA-15 with 3.3 nm mean pore radius has been studied photometrically for aqueous solutions containing a single protein type and for binary protein mixtures. Distinct variations in the absolute and relative adsorption behaviour are observed as a function of the solution's pH-value, and thus pore wall and protein charge. The proteins exhibit the strongest binding below their isoelectric points, which indicates the dominance of electrostatic interactions between charged amino acid residues and the -OH groups of the silica surface in the nanopore adsorption process. Moreover, we find for competitive adsorption in the restricted, tubular nano pore geometry that the protein type which shows the favoured binding to the pore wall can entirely suppress the adsorption of the species with lower binding affinity, even though the latter would adsorb quite well from a single component mixture devoid of the strongly binding protein. We demonstrate that this different electrochemical behaviour along with the large specific surface and thus adsorption capability of the nanoporous glass can be readily exploited for a simple, yet highly effective separation of protein mixtures by adjusting the aqueous solution's pH.

BP 17.18   Mon 17:30   Poster A
Rate equations as a tool for kinetic modelling of iRFP's — •Mario Willoweit, Nico Herder, Luisa Sauthof, Neslihan Tavraz, Franz-Josef Schmitt, and Thomas Friedrich — Institute of Chemistry, Bioenergetics, Technical University Berlin, Germany

Recent developments in protein design led to a near infrared fluorescent protein (iRFP) based on a bacteriophytochrome RpBphP2 (P2). Switchable infrared fluorescent probes with enhanced fluorescence quantum yield are required for modern microscopic applications like IR fluorescence microscopy. We investigated low-temperature time- and wavelength-correlated single photon counting in the wide temperature range from 10 K to 300 K to monitor chromophore-protein interactions. A rate equation model assuming ground state heterogeneity and three excited states: PR*, pre-Lumi-R* and Lumi-R* leads to the corresponding temperature-dependent rate constants and therefore a better understanding of the underlying pigment-protein coupling and the apparent fluorescent states in the system. The results enable to identify the molecular determinants for the fluorescence enhancement of iRFP compared to the wild-type protein. It is suggested that the mutations P2 D202T and P2 Y258F are mainly responsible for enhanced fluorescence quantum yield.

BP 17.19   Mon 17:30   Poster A
CUDA-accelerated FEM-BEM Simulations of Dielectric Relaxation Spectroscopy of solvated Proteins — •Stephan Kramer — Max-Planck-Institut f. biophysikalische Chemie, Am Faßberg 11, 37077 Göttingen

Dielectric relaxation spectroscopy of solvated ubiquitin [1] has shown the sensitivity of the direct current to conformational sampling. Experimentally, this is observed by the appearance of the so-called sub-β peak in the dielectric loss spectrum. A mechanistic explanation of this peak is that different numbers of ions are bound in the hydration shell of the protein, depending on its conformation. This changes the density of mobile ions, thus altering the direct current component. The sub-β peak can be quantified by a stochastic model considering the conformational dynamics as a simple 2-state, ratchet-like process coupled to a Fokker-Planck model for the mobile ions.

We extend the ion dynamics to the Poisson-Nernst-Planck equations in a finite domain with reactive boundaries modeling the setup of a dielectric relaxation spectroscopy experiment. The protein is an excluded volume for the ions. It is converted into a boundary condition for the mobile ions by means of an integral equation. The resulting boundary element problem is solved with CUDA using our SciPAL library [2]. The ion densities are computed from a finite element model. Our results confirm the theory of the origin of the sub-β peak.

[1] Ban et al. Angew. Chem. Int Ed., 50(48):11437-11440, 2011.
[2] S. C. Kramer and J. Hagemann, ACM TOPC (to appear), https://code.google.com/p/scipal/

BP 17.20   Mon 17:30   Poster A

Time-resolved single-frequency IR absorption spectroscopy on photosystem II for investigation of electron-coupled proton transfer — •Philipp Simon, Petko Chernev, and Holger Dau — Freie Universität Berlin, Fachbereich Physik

Photosystem II is a light activated and transmembrane protein performing photosynthetic water oxidation. During the accumulation of four oxidizing equivalents needed for O-O bond formation at the reaction center, a Mn_4Ca-oxo cluster, protons are released and transported over large distances of up to 30 Å(Klaus et al. 2012, PNAS 109, 16035-16040).

Understanding of the process at an atomic level does not only answer fundamental questions of protein functions but can also provide hints on the development of catalysts for artificial photosynthesis, a clean way of producing storable energy.

To analyse the dynamics of these processes a new infra-red absorption experiment is being designed. Its central part is a cw quantum-cascade laser tunable from 1300 to 1650 cm^{-1} and thus covering the amide I and II regions, the COO^- stretching region as well as bands of the quinones or the redox active tyrosine denoted as Y_Z. The time resolution is in the microsecond range, which enables us to observe structural changes and proton transfer dynamics. Here the setup and first measurements on the dynamics of selected vibrational bands, specifically the band assignable to Q_A, will be presented.

BP 17.21   Mon 17:30   Poster A

Single-molecule stochastic modeling of the channeling enzyme tryptophan synthase — •Dimitri Loutchko and Alexander S. Mikhailov — Fritz Haber Institute of the Max Planck Society

The channeling enzyme tryptophan synthase provides a paradigmatic example of a chemical nanomachine. It possesses two active centers and, as a single molecule, catalyzes a sequence of 13 different reactions with a complex pattern of allosteric regulation and with an intermediate product channeled from one active center to another. Here, the first single-molecule stochastic model of the enzyme is proposed and analyzed. All its transition rate constants were deduced from the experimental data available and no fitting parameters were thus employed. Numerical simulations reveal the development of strong correlations in the states of the active centers and the emergent synchronization of intramolecular processes in tryptophan synthase. While performed for a specific enzyme, this study sets a framework for stochastic modeling of other chemical machines, such as channeling enzymes and multi-enzyme complexes.

BP 17.22   Mon 17:30   Poster A

Free Energy Decomposition: A Model System with Focus on Entropic Contributions of Water — •Jonas Landsgesell and Jens Smiatek — Stuttgart

This contribution focuses on the application of free energy decomposition to investigate the entropic contributions of water to the folding of the beta hairpin HP7 and its mutants by simulations in explicit water and vacuum. Free energy decomposition makes use of free energy landscapes which are obtained using all-atom molecular dynamics simulations together with umbrella sampling and WHAM. The chosen methods calculate entropy changes by using internal energy and free energy estimates. In agreement with experiments we find that the folding of the beta hairpin HP7 is mainly driven by enthalpic energy changes. The simulations of some mutants of HP7 show that the influence of the hydrophobic effect on protein folding can be increased by replacing less hydrophobic amino acids with more hydrophobic amino acids.