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Book of Abstracts

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EMBL



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Speakers' abstracts

Philip Anfinrud (National Institutes of Health, Bethesda, MD)

Picosecond Photobiology: Watching a Signaling Protein Function in Real Time via 150 Picosecond Time-Resolved X-ray Diffraction and Solution Scattering

To understand how signaling proteins function, it is crucial to know the time-ordered sequence of events that lead to the signaling state. We recently developed on the BioCARS beamline at the Advanced Photon Source the infrastructure required to characterize structural changes in proteins, and have used this capability to track the reversible photocycle of photoactive yellow protein following trans-to-cis photoisomerization of its p-coumaric acid (pCA) chromophore. Briefly, a picosecond laser pulse photoexcites pCA and triggers a structural change in the protein, which is probed with a suitably delayed picosecond X-ray pulse. When the protein is studied in a crystalline state, this “pump-probe” approach recovers time-resolved diffraction “snapshots” whose corresponding electron density maps can be stitched together into a real-time movie of the structural changes that ensue. However, the actual signaling state is not accessible in the crystalline state due to crystal packing constraints. This state is accessible in time-resolved small- and wide-angle X-ray scattering studies, which probe changes in the size, shape, and structure of the protein. The mechanistically detailed, near-atomic resolution description of the complete PYP photocycle developed from these studies provides a framework for understanding signal transduction in proteins, and for assessing and validating theoretical/computational approaches in protein biophysics. This research was supported in part by the Intramural Research Program of the NIH, NIDDK.

Jean Dalibard (Département de Physique de l'École Normale Supérieure, Paris, France)

Bose-Einstein condensates and antiferromagnetic interactions:

An Illustration of symmetry breaking in Quantum Mechanics

In a spinor Bose gas, contact interactions can induce effective spin-spin interactions [1]. In the case of sodium atoms (^{23}Na , spin 1), these effective interactions are antiferromagnetic, which leads to a series of interesting phenomena. Here I will focus on recent experimental investigations that we have performed at ENS on a sodium condensate in the so-called *Single Mode Approximation* [2]: in this low temperature regime, all atoms occupy the same orbital wave function and only the spin degree of freedom is relevant. In the absence of external field, the exact ground state is expected to be the (massively entangled) singlet state, with a zero total spin [3]. However one can also use an approximate symmetry-breaking approach, in which all atoms condense a single spin state $S_z=0$ along an arbitrary z direction. I will discuss both approaches and connect them with the notion of a *fragmented condensate* [4], i.e., a situation where several states of a many-body system are simultaneously macroscopically populated [5].

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William A. Eaton (National Institutes of Health, Bethesda)

Toward observing transition paths in protein folding by single molecule fluorescence

The transition-path is the tiny fraction of an equilibrium, single-molecule trajectory when a transition occurs between two states. The importance of the transition-path in protein folding is that it contains all the mechanistic information on how a protein folds and unfolds, explaining why it is currently being studied extensively by all-atom molecular dynamics simulations and theoretical analysis of these simulations. However, a transition-path has never been observed experimentally for any molecular system in the condensed phase. Because it is a single molecule property, even determining the average transition-path time is challenging. In this presentation I will discuss how we use measurements of Foerster resonance energy transfer in single molecule fluorescence experiments and a photon-by-photon analysis to measure average transition path times for proteins of different topology and folding speed using the Gopich/Szabo maximum likelihood method. I will also present our latest results on how transition path times as a function of temperature and viscosity characterize the diffusion coefficient of Kramers theory. These results are just the first, but important, steps toward measuring intra-molecular distances during individual transition paths, which should provide the most demanding tests of both theoretical models and simulations of protein folding.

**This work is done in collaboration with Hoi Sung Chung.*

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Petra Fromme (University of Arizona, Tucson, USA)

Time-Resolved Femtosecond Nanocrystallography of membrane proteins opens a new Era in Structural Biology

Petra Fromme,¹ Christopher Kupitz,¹ Shibom Basu,¹ Ingo Grotjohann,¹ Raimund Fromme,¹ Henry Chapman, DESY³, Anton Barty,³ Thomas A. White³, Daniel P. DePonte,^{1,3,4}, Richard. A. Kirian,³ Mark S. Hunter⁶, Mathias Frank⁶, Kimberley Rendek,¹ Nadia Zatespin,² JayHow Yang,¹ Jesse Bergkamp,¹ Haiguang Liu,² Daniel James,² Dingjie Wang,² Ilme Schlichting,⁴, Robert Shoeman,⁴, Sébastien Boutet,⁵ Garth Williams,⁵ Kevin Schmidt,² Herve Bottin, CEA⁷, R. Bruce Doak,² Uwe Weierstall,² John.C.H. Spence,² (see refs (1-3) for additional authors)

1, Arizona State University, Department of Chemistry and Biochemistry, Tempe, USA, 2, Arizona State University, Department of Physics Tempe, USA, 3, Center for Free-Electron Laser Science, DESY, 22607 Hamburg, Germany and University of Hamburg, 22761 Hamburg, Germany, 4. Max Planck Advanced Study Group, Center for Free Electron Laser Science (CFEL), 22607 Hamburg, Germany and Max-Planck-Institut für medizinische Forschung, 69120 Heidelberg, Germany, 5. LCLS, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA, Stanford PULSE Institute, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA., 6. Lawrence Livermore National Lab, 7. CEA Saclay, France

Femtosecond nanocrystallography provides a novel concept for structure determination, where X-ray diffraction “snapshots” are collected from a fully hydrated stream of nanocrystals, using femtosecond pulses from the world's first high energy X-ray free-electron laser, the Linac Coherent Light Source. Photosystem I, which is the most complex membrane that has been crystallized to date, consisting of 36 proteins and 381 cofactors, was used as the model system. The experiments show the proof of concept that diffraction of nanocrystals that contain only 100-10 000 Photosystem I molecules can be observed using femtosecond pulses that are 10^{12} stronger than 3rd generation synchrotron sources and destroy any material that is placed in its focus. Over 3 million diffraction patterns from individual nanocrystals (100nm- 2 μ m in size) were collected and evaluated [1]. By using femtosecond pulses briefer than the time-scale of most damage processes, femtosecond nanocrystallography overcomes the problem of X-ray damage in crystallography. Data collected at the new CXI LCLS beamline at higher energy (8keV) showed that the concept of fs crystallography extends to atomic resolution [2]. Our first novel structure solved with fs crystallography was highlighted in Science as one of the 10 breakthroughs of the year [3]. Data will be presented that show that nanocrystals of membrane proteins, which are notoriously difficult to crystallize, have extremely low mosaicity. Femtosecond crystallography also opens a new avenue for determination of protein dynamics. First experiments on time resolved X-ray crystallography have been performed on Photosystem I-ferredoxin and Photosystem II nano-crystals. The first results are very promising and pave the way for a new avenue in X-ray crystallography that may allow the determination of molecular movies of the dynamics of membrane proteins "at work" in the future including the determination of a molecular movies of water splitting.

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TRM Barends, R Neutze, S Marchesini, R Fromme, S Schorb, D Rupp, M Adolph, T Gorkhovev, I Andersson, H Hirsemann, G Potdevin, H Graafsma, B Nilsson, and JCH Spence "Femtosecond x-ray protein nanocrystallography", *Nature*, 470, 73-77

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Acknowledgement: Experiments were carried out at the Linac Coherent Light Source and the Advanced Light Source, operated by Stanford University and the University of California (respectively) on behalf of the U.S. Department of Energy (DOE), Office of Basic Energy Sciences. We acknowledge support from DOE through the PULSE Institute at the SLAC National Accelerator Laboratory and by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, the National Institute of Health (award 1R01GM095583-01), the National Science Foundation (awards 0417142 and 1021557), the Helmholtz Association, the Max Planck Society for funding the development and operation of the CAMP instrument, P.F. was partially supported by the Center for Bio-Inspired Solar Fuel Production, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001016.

Rienk van Grondelle (Vrije Universiteit Amsterdam, Netherlands)

The Quantum Design of Photosynthesis

Photosynthesis has found an ultrafast and highly efficient way of converting the energy of the sun into electrochemical energy. The solar energy is collected by Light-Harvesting complexes (LHC) and then transferred to the Reaction Center (RC) where the excitation energy is converted into a charge separated state with almost 100% efficiency. That separation of charges creates an electrochemical gradient across the photosynthetic membrane which ultimately powers the photosynthetic organism. The understanding of the molecular mechanisms of light harvesting and charge separation will provide a template for the design of efficient artificial solar energy conversion systems.

Upon excitation of the photosynthetic system the energy is delocalized over several cofactors creating collective excited states (excitons) that provide efficient and ultrafast paths energy transfer using the principles of quantum mechanics. In the reaction center the excitons become mixed with charge transfer (CT) character (exciton-CT states), which provide ultrafast channels for charge transfer. However, both the LHC and the RC have to cope with a counter effect: disorder. The slow protein motions (static disorder) produce slightly different conformations which, in turn, modulate the energy of the exciton-CT states. In this scenario, in some of the LHC/RC complexes within the sample ensemble the energy could be trapped in some unproductive states leading to unacceptable energy losses.

Here I will show that LHCs and RCs have found a unique solution for overcoming this barrier: they use the principles of quantum mechanics to probe many possible pathways at the same time and to

select the most efficient one that fits their realization of the disorder. They use electronic coherence for ultrafast energy and electron transfer and have selected specific vibrations to sustain those coherences. In this way photosynthetic energy transfer and charge separation have achieved their amazing efficiency. At the same time these same interactions are used to photoprotect the system against unwanted byproducts of light harvesting and charge separation at high light intensities.

Walter Kob (Université de Montpellier, France)

Influence of the glass transition on the liquid-gas spinodal decomposition

Gels are disordered systems that we encounter in our daily life in a variety of forms, such as glues, contact lenses, cosmetics, in electrophoresis, etc. The presence of their intrinsic disorder allows to strongly modify their properties, but also makes their theoretical description a big challenge. In this talk I will focus on a particular type of gel: Those that have been created by quenching a glass-forming liquid into its coexistence region and thus will undergo a phase separation which makes that the structure becomes nonergodic. I will present the results of computer simulations of a simple glass-former that does indeed form a gel under these conditions and discuss methods how the resulting disordered structure can be characterized. Subsequently I will show how the aging dynamics affects the properties of this coarsening system.

Thomas Kühne (Johannes Gutenberg Universität Mainz, Germany)

Microscopic properties of liquid water from combined ab initio molecular dynamics and energy decomposition studies

A new energy decomposition analysis for periodic systems based on absolutely localized molecular orbitals is presented [1, 2]. In combination with the recently developed "Car-Parrinello-like approach to Born-Oppenheimer MD" [3] this not only allows for ab initio molecular dynamics simulations on previously inaccessible time and length scales, but also provide unprecedented insights into the nature of hydrogen bonding between water molecules. However, in contrast to the original scheme, large integration time steps can be used. By this means the best of the Born-Oppenheimer and the Car-Parrinello methods are unified, which not only extends the scope of either approach, but allows for ab initio simulations previously thought not feasible. The effectiveness of this new combined Approach is demonstrated on liquid water and the water/air interface [4, 5]. Our simulations reveal that although a water molecule forms, on average, two strong donor and two strong acceptor bonds, there is a significant asymmetry in the energy of these contacts. We demonstrate that this asymmetry is a result of small instantaneous distortions of hydrogen bonds and show that the distinct features of the X-ray absorption spectra originate from molecules with high instantaneous asymmetry [1, 2, 6, 7].

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Rick Millane (University of Canterbury, New Zealand)

Molecular imaging using x-ray free-electron laser diffraction by nanocrystals

X-ray free-electron lasers (XFELs) offer unprecedented opportunities for imaging of extremely small specimens. One of these opportunities is in protein x-ray crystallography, since the use of XFELs can overcome the necessity of growing of macroscopic crystalline specimens, and radiation damage can be circumvented by the x-ray pulse terminating before significant damage occurs. XFEL diffraction data from protein nanocrystals, however, have some different characteristics to those in conventional protein x-ray crystallography. These characteristics require novel data processing and image reconstruction algorithms. In this talk I will review the background to XFEL nanocrystallography, and describe some of the considerations and methods used for image reconstruction.

Tilman Pfau (Physikalisches Institut, Universität Stuttgart, Germany)

How electrons catch ground state atoms

Electrons attract polarizable atoms via a $1/r^4$ potential. For slow electrons the scattering from that potential is purely s-wave and can be described by a Fermi pseudopotential. To study this interaction Rydberg electrons are well suited as they are slow and trapped by the charged nucleus. In the environment of a high pressure discharge Amaldi and Segre, already in 1934 observed a lineshift proportional to the scattering length [1], which was first introduced to explain their findings.

At ultracold temperatures and Rydberg states with medium size principle quantum numbers n , one or two ground state atoms can be trapped in the meanfield potential created by the Rydberg electron, leading to so called ultra-long range Rydberg molecules [2]. These molecules can show a linear Stark effect corresponding to a permanent dipole moment [3], which if seen from a standpoint of traditional molecular physics is surprising.

At higher Rydberg states the spatial extent of the Rydberg electron orbit is increasing. For principal quantum numbers n in the range of 100-200 and typical BEC densities, up to several ten thousand ground state atoms are located inside one Rydberg atom, leading again to a density dependent energy shift of the Rydberg state. This allows, together with the strong van-der-Waals blockade, to excite only one single Rydberg atom in a condensate. We excite a Rydberg electron with n upto 202 in the BEC, the size of which becomes comparable to the size of the BEC. We study their life time in the BEC and the coupling between the electron and phonons in the BEC [3]. So the single electron that we prepare in a quantum gas allows nicely to study the transition from two- to few- to many-body interaction.

As an outlook, the trapping of a full condensate inside a Rydberg atom of high principal quantum number and the imaging of the Rydberg electron's wavefunction by its impact onto the surrounding ultracold cloud seem to be within reach.

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Hossein Sadeghpour (ITAMP, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts, USA)

Dynamics in large carbon-rich structures: how the first carbon molecules may have synthesized in interstellar space

Carbon is the 4th most abundant element in the Universe. It is the building block of life. Hydrocarbons, alcohols, acids, aldehydes, amines, and sugar have been detected in interstellar medium (ISM). There's substantial evidence pointing to the existence of polycyclic aromatic hydrocarbons (PAHs) in space. Vibrational lines of fullerenes (otherwise known as footballs) have been detected in the microwave in nebulae. The mere fact that such atomistically pristine molecules are now known to exist in the dust of the ISM, while their natural terrestrial abundance is low, raises fascinating challenges. Where do they come from? How are they synthesized? What are the dynamics leading to self-assembly and what are the rates for such reactions? In this presentation, I will attempt at addressing some of these questions.

Jonathan Tennyson (University College London, UK)

R-matrix calculations of electron molecule (re-) collisions

The R-matrix method provides a comprehensive framework for treating the electron-molecule collision problem [1]. It is being used to characterise the electron -- molecular ion collision problem with unprecedented detail by treating both bound and continuum states using the same computational models [2]. This work is currently being extended to photoionisation problems by implementing a time-dependent approach based on those developed to treat atomic problems by the Belfast group. Progress on this work will be discussed at the meeting.

1. J. Tennyson,

Electron - molecule collision calculations using the R-matrix method@@,

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Posters

Betz, Thomas

Dzemiantsova, Liudmila

Spin sensitivity and Spin dynamics in magnetic nanostructures via nuclear resonance spectroscopy

Chang, Y.-P.; Dlugolecki, K.; Küpper, J.; Rösch, D.; Wild, D.; Willitsch, S.

Specific Chemical Reactivities of Spatially Separated 3-aminophenol Conformers with Cold Ca⁺ Ions

Grenda, Neele

Local probes for light-driven intra-molecular charge transfer

Jurek, Zoltan

Lehmkuhler, Felix

Structure and Dynamics of Glass-forming Colloidal Suspensions

Li, Zheng

Electron-hole dynamics after valence photoionization

Mietner, Benedikt

Strukturelle und thermodynamische Untersuchungen zum Phasenverhalten von Wasser in geordneten nanoporösen Wirtstrukturen mit unterschiedlichen Oberflächenpolaritäten /

Structural and thermodynamic studies on the phase behavior of water in ordered, nanoporous host structures with different surface polarities

Mullins, Terry; Trippel, Sebastian; Müller, Nele; Kienitz, Jens; Küpper, Jochen

Alignment of state-selected OCS: Rotational dynamics and the complete determination of the molecular eigenstate

Nalbach, Peter

Photosynthetic energy transfer in green sulfur bacteria

Perbandt, Markus

Designing time-resolved X-ray crystallography experiments applying photolysis of caged compounds in combination with serial crystallography

Redder, Tobias

X-ray diffraction of growing gold nanoparticles

Ruff, Bernhard

Imaging local and global coherences of superfluid matter -- Dynamics and Control of quantum matter

Singh, Vijay Pal

Noise correlations and superfluid behavior of 2D Bose gases

Son, Sang-Kil

XATOM: an integrated toolkit for X-ray and atomic physics

Steinke, Ingo

Liquid jets for Experiments on Molecular liquids

Trippel, Sebastian; Mullins, Terry; Müller, Nele; Kienitz, Jens; Küpper, Jochen

Pendular-state wavepacket dynamics and non-adiabatic effects of state-selected OCS molecules

Vendrell, Oriol