The Journal of Chemical Physics

Future of Chemical Physics

31 August to 2 September, 2016

St. Edmund Hall
University of Oxford
Oxford, United Kingdom
Future of Chemical Physics

**Date:** 31 August – 2 September, 2016

**Location:** St. Edmund Hall, University of Oxford, Oxford, United Kingdom

**Conference Organizers:**
- Angelos Michaelides (University College London), Associate Editor, JCP
- David Manolopoulos (University of Oxford), Deputy Editor, JCP
- Peter Hamm (University of Zurich), Deputy Editor, JCP
- Carlos Vega (University Complutense of Madrid), Associate Editor, JCP
- Marsha I. Lester (University of Pennsylvania), Editor in Chief, JCP

Future of Chemical Physics is an AIP Publishing Horizons conference sponsored by The Journal of Chemical Physics (JCP). Designed to facilitate conversation between innovative researchers at the forefront of chemical physics, this inaugural conference will help shape the future of the field.

Please contact Erinn Brigham, Asst. Journal Manager for JCP, at ebrigham@aip.org with any questions or concerns throughout and after the conference. For urgent matters call +1.352.870.4211.

**Wednesday 31 August**

9:00 - 13:00 Registration in St. Edmund Hall
13:45 - 14:00 Welcome and opening remarks - Marsha I. Lester (PTCL)

**Session I: Atoms, Molecules and Clusters (Chair: David W. Chandler)**
14:00 Andre Fielicke (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Shedding IR light on gas-phase metal clusters: insights into structures and reactions
14:30 Jonathan Reid (University of Bristol)
Challenges in the chemical physics of aerosols
15:00 Claire Vallance (University of Oxford)
State-of-the-art imaging techniques for chemical dynamics studies
15:30 - 16:00 Coffee and tea break

**Session II: Liquids, Glasses, and Crystals (Chair: Jeppe Dyre)**
16:00 Ludovic Berthier (Université de Montpellier)
Facets of glass physics
16:30 Kristine Niss (Roskilde University)
Is the glass transition universal?
17:00 Sylvie Roke (École Polytechnique Fédérale de Lausanne)
Aqueous nanoscopic systems
18:00 - 19:30 Poster session I
19:30 - 21:30 Dinner
21:30 - Welcome Mixer in Bar

**Thursday 1 September**

**Session III: Surfaces, Interfaces and Materials (Chair: Angelos Michaelides)**
8:30 Natalie Banerji (University of Fribourg)
Uncovering the photophysics of organic and hybrid semiconductors
9:00 Susan Perkin (University of Oxford)
Ionic liquids—a challenge to our understanding of the liquid state
9:30 Aron Walsh (University of Bath)
Disorder, defects and temperature: Modelling real materials from first-principles
10:00 - 10:30 Coffee and tea break

**Session IV: Polymers and Soft Matter (Chair: Carlos Vega)**
10:30 Dirk Aarts (University of Oxford)
Directed self-assembly of Janus rods
11:00 Joachim Dzubiella (Helmholtz-Zentrum Berlin)
Multiscale modeling of soft functional materials based on responsive polymers: towards adaptivity and feedback control
11:30 Friederike Schmid (Johannes Gutenberg Universität Mainz)
Surface design with polymers
12:30 - 13:30 Lunch

horizons.aip.org/future_chemical_physics.htm
Thursday 1 September continued

Session V: Biological Molecules and Networks (Chair: James T. (Casey) Hynes)
14:00 - 14:30  Damien Laage (École Normale Supérieure)
Biophysical hydration shells: dynamics and biochemical function
14:30 - 15:00  Ben Schuler (University of Zurich)
Biophysics at the nanoscale: Single-molecule spectroscopy of protein folding and dynamics
15:00 - 15:30  Birgit Strodel (Forschungszentrum Jülich)
Advances in the simulation of protein aggregation at the atomistic scale
15:30 - 16:00  Coffee and tea break

Session VI: Advanced Experimental Techniques (Chair: Peter Hamm)
16:00 - 16:30  Sharon Ashbrook (University of St. Andrews)
Investigating structure using solid-state NMR: Principles, state-of-the-art and challenges
16:30 - 17:00  Niek F. van Hulst (ICFO – the Institute of Photonic Sciences)
Pushing chemical physics to the nanoscale
17:00 - 17:30  Philipp Kukura (University of Oxford)
Femtosecond time-resolved microspectroscopy
18:00 - 19:30  Poster session II
19:30 - 21:30  Conference Dinner

Friday 2 September

Session VII: Theoretical Methods and Algorithms (Chair: Sotiris Xantheas)
9:00 - 9:30  Michele Ceriotti (École Polytechnique Fédérale de Lausanne)
Using machine learning to map the structure and predict the properties of materials and molecules
9:30 - 10:00  Fred Manby (University of Bristol)
Quantum electrodynamics of the early stages of photosynthetic light absorption
10:00 - 10:30  Ali Alavi (University of Cambridge/MPI for Solid State Research)
New directions for Monte Carlo algorithms in electronic structure theory: FCI, CASSCF and multi-reference perturbation theory
10:30 - 11:00  Coffee and tea break

Session VIII: Future of Chemical Physics (Chair: David Manolopoulos)
11:00 - 11:30  Panel Discussion: The Future of Chemical Physics
Panelists:
Jeppe Dyre (Roskilde University)
Thomas Elsaesser (Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie)
James T. (Casey) Hynes (University of Colorado Boulder, École Normale Supérieure)
David H. Parker (Radboud University)
Michele Parrinello (ETH Zurich)
11:30 - 12:00  Announcement of the poster prizes and closing remarks
(Marsha I. Lester)
12:00 - 12:30  Adjourn

Sharon E. Ashbrook
Professor, University of St. Andrews

PRESENTATION TITLE:
Investigating structure using solid-state NMR: Principles, state-of-the-art and challenges

ABSTRACT
Nuclear Magnetic Resonance (NMR) spectroscopy is one of the most widely-used analytical tools in chemistry and is one of the most powerful. As practically all elements in the periodic table can be studied using NMR, the technique has been used in wide-ranging areas such as materials science, geochemistry, biology and medicine. The ability of NMR to obtain detailed local structural information, without relying on any long-range order, has resulted in the relatively recent development of NMR as an important method for the study of solids. However, NMR spectra of solids contain much broader lines than in solution (as a result of the orientation-dependent nature of the interactions affecting the nuclear spins, which are averaged in solution by rapid tumbling), making it difficult to separate signals and extract the information required. In recent years, there has been growing interest in the experimental community in the use of first-principles calculations, i.e., the computational prediction of NMR parameters for a specified structural model, in order to aid spectral interpretation and assignment. The application of theoretical calculations for solids was revolutionised in 2001 through the introduction of the gauge-including projector augmented wave (GIPAW) approach, which enabled the calculation of magnetic shielding in a periodic system.

While the uses of materials depend upon their bulk properties, the first step in understanding how these arise is to determine the local environment of the atoms within a structure. The sensitivity of NMR spectroscopy to small changes in the local environment makes it a powerful tool for the characterisation of solids. This talk will discuss the ongoing quest to improve resolution and sensitivity in NMR spectroscopy and the recent opportunities to exploit theoretical calculations alongside experimental measurement to aid analysis. The current state-of-the-art in experiment and theory will be described, and the possibilities for future improvements and advances considered.

BIOSKETCH
Sharon Ashbrook (b. 1975) is a Professor of Physical Chemistry at the University of St Andrews. Following a DPhil at the University of Oxford (2001), she completed postdoctoral work at the University of Exeter, before being awarded a Royal Society Dorothy Hodgkin Fellowship (2003) which she held at the University of Cambridge. During this time she also held the Charles and Katherine Darwin Research Fellowship at Darwin College. From October 2005, she was appointed as an RCUK Academic Fellow in the School of Chemistry at the University of St. Andrews, and was promoted to Reader in 2009 and Professor in 2013.

Her research focuses on the application of multinuclear solid-state NMR spectroscopy techniques and most recently, their combination with first-principles DFT calculations to investigate structure, disorder and dynamics in the solid state. She has published over 130 journal articles and 5 book chapters in this area. She was awarded the RSC Harrison Prize (2004), Marlow Award (2011) and Corday Morgan Prize (2015) and the RSE MacDougall Brisbane Medal (2012). She holds a Wolfson Merit Award and an ERC Consolidator Grant and was elected FRSE in 2016. She was a member of the 2014 Hong Kong Physical Sciences RAE panel.
ABSTRACT
Physical and theoretical chemists appear to have a remarkable ability to defy the exponential increase of available computer power by incrementing the complexity of their models at an even faster pace. On the bright side, this process is making predictive modelling of materials and molecules a reality, but at the same time the sheer amount of data produced by simulations, as well as their intrinsic complexity, makes it extracting physical insight from the models a challenge of its own.

In this talk I will discuss how computers can help us facing this challenge, leveraging machine-learning algorithms that are at the core of modern data science. The crucial ingredient in applying these algorithms to chemistry and materials lies in providing a robust mathematical translation of the notion of chemical similarity. I will focus in particular on how one can introduce an effective metric to compare structures. I will then demonstrate how such an (al)chemical similarity measure can be used as the basis for building intuitive maps of chemical landscapes, as well as to predict physical-chemical properties without relying on expensive quantum chemical calculations.

BIOSKETCH
Michele Ceriotti received his Ph.D. in Physics from ETH Zurich, under the supervision of Prof. Michele Parrinello. He was then awarded a Swiss National Science Foundation postgraduate fellowship, as well as a Royal Society Newton International Fellowship and a Marie Curie Intra-European Fellowship, with which he spent three years in Oxford in the Physical and Theoretical Chemistry Laboratory, working with Prof. David E. Manolopoulos. During his time in Oxford, he was also appointed as a Junior Research Fellow at Merton College. Since November 2013 he works as an assistant professor at the Institute of Materials at EPFL Lausanne, where he leads the laboratory for Computational Science and Modelling. His research interests focus on the development of methods for molecular dynamics and the simulation of complex systems at the atomistic level, and to their application to problems in chemistry and materials science—ranging from accelerated techniques to model nuclear quantum effects to machine-learning techniques to analyse and predict the properties of materials and molecules.

ABSTRACT
The physical basis for efficient energy transport in photosynthesis has been the subject of intense research for many decades now. Experimentation has revealed the beautiful structural biology of the light-harvesting machinery, as well as a wealth of data on the dynamics of energy transport. Much theoretical and computational work has focused on the role of static disorder and dynamical coupling to environment modes in shaping the phenomenology of energy transport. Here I will focus on another aspect of photosynthesis, namely the role of the state of the incident radiation from the sun, and the nature of the excitation formed in the light-harvesting apparatus. This is just one element of a wider effort in our group to construct unified quantum models of the joint system composed of radiation, chromophores and bath modes.

BIOSKETCH
Fred Manby is a Professor of Theoretical Chemistry at the University of Bristol, and Co-Director of the EPSRC Centre for Doctoral Training on Theory and Modelling in Chemical Sciences. He took his first degree and PhD at the University of York, before working as a postdoc with Professor Peter Knowles in the University of Birmingham. He was awarded a Royal Society University Research Fellowship, which he took up at the University of Bristol in 2000. His research is mainly in the fields of quantum chemistry and method developments in electronic structure theory.
Claire Vallance  
Professor of Physical Chemistry, University of Oxford  

**ABSTRACT**  
Over the past three decades, ion imaging and velocity-mapping techniques have truly captured the imagination of the reaction dynamics community. Such methods provide a visual snapshot of the complete product scattering distribution following a reactive event, revealing the kinetic energy, angular, and internal energy distributions of the newly formed products and providing unparalleled insight into the detailed dynamics of the process under study. Such methods have contributed enormously to our ability to understand the underlying ‘physics’ that controls chemical reactivity.

Recent developments in ultrafast image sensor technology have further extended the scope of velocity-map imaging methods. When coupled with universal ionization methods, the ability of the new sensors to image multiple fragments within a single experiment allows the study of larger and more complex systems, which often possess multiple distinct product pathways. Such sensors also offer a number of fundamentally new capabilities in areas such as coincidence detection, allowing correlated distributions of two or more fragments to be recorded.  We will review the current status of ultrafast image sensor technology in the context of reaction dynamics experiments, providing examples of recent applications, before discussing potential future developments.

**BIOSKETCH**  
Claire Vallance is a Professor of Physical Chemistry in the Department of Chemistry at the University of Oxford, and Tutorial Fellow in Physical Chemistry at Hertford College. After graduating with B.Sc (hons) and Ph.D degrees from the University of Canterbury (in Christchurch, New Zealand), she moved to Oxford in 1999 to take up a three-year Glasstone Research Fellowship in the Physical and Theoretical Chemistry Laboratory. She then held a Royal Society University Research Fellowship in the same department for two years, before she was appointed to a University Lectureship in 2005. She became a full professor in 2013.

Claire’s current research interests include reaction dynamics, applications of velocity-map and spatial-map imaging to mass spectrometry, and the development of laser spectroscopy techniques for microfluidics and chemical sensing applications. She has authored or co-authored around 90 research papers, invited reviews, and book chapters in these areas, as well as co-editing the textbook Tutorials in Molecular Reaction Dynamics, published in 2010. A second textbook, Astrochemistry from the Big Bang to the Present Day, will be published in the summer of 2016.

Jonathan P. Reid  
Professor, University of Bristol  

**ABSTRACT**  
Particles dispersed in a gas phase present many challenges for experimental investigation. Spanning a wide range in size (from the nanometre to the 10’s of micrometres scale), processes can occur over a time period spanning from nanoseconds to days. When considered in combination, addressing these challenges of lengthscale and timescale is key to understanding the richness of their behaviour and their application in fields as diverse as drug delivery to the lungs, the atomisation of fuels, the drying of formulated sprays, the transmission of airborne pathogens and their atmospheric chemistry. Although conventional techniques are mostly only able to provide measurements of average properties (both over size and time), novel single particle techniques can allow detailed measurements and provide unparalleled resolution of the processes central to understanding the chemical physics of aerosols.

We will begin by reviewing many of the new tools available for interrogating the properties of individual airborne particles, including optical and electrodynamic traps for manipulating a single particle or an array, and linear and nonlinear spectroscopies. We will then briefly explore how these tools can be used to provide insight into some of the key challenges faced in understanding aerosol, specifically: surface tension and condensational growth kinetics, bulk viscosity, phase behaviour and molecular diffusion; heterogeneous chemistry and confined environments; and the viability of bacteria and viruses in the aerosol phase. In each example, we will consider the benefits of detailed metrology and how rigorous studies in chemical physics can address the challenges faced in important fields of application.

**BIOSKETCH**  
Jonathan Reid is Professor of Physical Chemistry at the University of Bristol. Following both undergraduate study and postgraduate research at the University of Oxford, he undertook a period of post-doctoral research at JILA at the University of Colorado, USA. He returned to the UK as a lecturer at the University of Birmingham, moving to Bristol in 2004, where he was promoted to Professor in 2009. He has held both EPSRC Advanced and Leadership Fellowships and has been the recipient of the Royal Society of Chemistry (RSC) Corday-Morgan medal (2013), the Marlow medal of the Faraday Division (2004) and the Harrison Memorial medal (2001). His research spans fields extending from atmospheric science to drug delivery to the lungs, the factors controlling the viability of bacteria and viruses in the aerosol phase, and the formulation science of aerosol. He has published over 140 publications in peer-reviewed journals, is on the editorial board of the RSC journal Chemical Society Reviews, is a Fellow of the RSC, and is vice-president of the Aerosol Society of UK and Ireland.
ABSTRACT
The physics associated with the glass transition control the dramatic evolution of transport coefficients in systems as diverse as dense liquids, polymers, colloids, but also granular particles and active matter. The canonical liquid-glass transition in equilibrium fluids is characterized by several phenomenological crossovers, but glasses are formed without crossing any sharp singularity. The glass problem has been an important research theme in chemical physics over many decades.

I will present results suggesting that equilibrium phase transitions relevant to the physics of highly viscous liquids can now be analysed using new theoretical and computational tools developed specifically for this venerable glass problem. These results should demonstrate that theoretical studies of the glass transition have entered a new phase, where the relevant order parameter and thermodynamic fluctuations can be directly probed, getting us closer to testing the existence of an equilibrium phase transition underlying the formation of glassy states. A solution to the glass problem from first principles thus appears to be within reach.

BIOSKETCH
Ludovic Berthier received his Ph-D in theoretical physics in 2001 from the École Normale Supérieure in Lyon, France. In 2002, he became a Marie Curie Postdoctoral Fellow at the Department of Theoretical Physics at Oxford University. In 2004 he was appointed as a CNRS research associate at the University of Montpellier, France. In 2007, he was a visiting scientist at the James Franck Institute of the University of Chicago, US. He is now CNRS research director in the Laboratoire Charles Coulomb at the University of Montpellier. He has published over 130 peer-reviewed articles on the topics of statistical mechanics of disordered materials, nonequilibrium phase transitions and soft matter using a combination of theoretical and computational methods.

ABSTRACT
Proteins are the most versatile constituents of the molecular machinery of life. Understanding their remarkable mechanisms of self-organization and their functional properties requires detailed knowledge of their structure and dynamics. Single-molecule spectroscopy provides an opportunity for investigating these properties on nanometer lengthscales and down to nanosecond timescales. Probing individual molecules can reveal structural and dynamic heterogeneity usually hidden in the ensemble average. Förster resonance energy transfer (FRET) combined with correlation spectroscopy, microfluidics, and the quantitative analysis of photon statistics enable us to probe the equilibrium and non-equilibrium dynamics of proteins, even in complex environments, including live cells. A physical description of biomolecular behavior is becoming accessible via the synergy of experiment with analytical theory and molecular simulations.

BIOSKETCH
Ben Schuler is Professor of Molecular Biophysics at the University of Zurich. He investigates the structure, dynamics, folding, and misfolding of proteins with biophysical methods, in particular single-molecule fluorescence. Ben Schuler studied Chemistry and Biochemistry at the University of Regensburg, Germany, and at the University of Kent, UK. He received his PhD in Physical Biochemistry from the University of Regensburg in 1998 and did his postdoctoral research in the Laboratory of Chemical Physics at the National Institutes of Health in Bethesda, USA. Ben Schuler then headed an independent research group at the University of Potsdam in Germany supported by the Emmy Noether Program of the Deutsche Forschungsgemeinschaft. He joined the University of Zurich as Assistant Professor in 2004 and was promoted to Full Professor in 2009.
ABSTRACT
Responsive polymer systems play a key role in the development of novel soft functional materials for future industrial and biotechnological applications. For those modern developments it becomes increasingly desirable that material function can adapt to the local environment and be tuned by internal feedback mechanisms. These high demands on novel functional properties pose major future challenges on systematic (multiscale) modeling approaches due to the complexities originating from spatio-temporal couplings over many length and time scales. One example discussed in this presentation is the rational design and optimization of responsive core-shell ‘nanoreactors’ [1-3]. In the latter, metal nanoparticles are stabilized in aqueous solution by an encapsulating thermosensitive hydrogel shell, containing and sheltering the reaction catalyzed by the nanoparticles. The physicochemical properties of the polymeric ‘gate’ respond to stimuli in the environment, which permits the reactant fluxes and the catalytic reaction to be switched and tuned, e.g., by the temperature, salt concentration, or solvent composition. Hence, the novel hybrid character of these emerging nanoreactors opens up unprecedented ways for the control of nanocatalysis and its adaption to the local environment, while strongly challenging future multiscale theory and simulations (from molecular-scale solvation interactions to macroscopic function) in nonequilibrium.


BIOSKETCH
Joachim Dzubiella received his doctorate in 2002 under the supervision of Prof. C. N. Likos and Prof. H. Löwen in Theoretical Soft Matter Physics at the Heinrich-Heine Universität in Düsseldorf, Germany. After postdoctoral stays with Prof. J.-P. Hansen in Cambridge, UK, and Prof. A. J. McCammon in San Diego, USA, he returned to Germany in 2006 to head an Emmy-Noether research group at the Technical University Munich. Since 2010 he is a group leader at the Helmholtz-Zentrum Berlin and Professor for Theoretical Physics at the Humboldt-Universität zu Berlin.

ABSTRACT
A real crystal can never be perfect, yet the majority of first-principles materials modelling is focused on pristine infinite crystals. The standard toolkit of solid-state chemistry and physics relies heavily on periodic functions, while it is the deviations and imperfections that often determine the physical properties of solids. In this talk, I will discuss progress in the theoretical description of imperfect solids from first-principles including thermal vibrations, point defects and the absence of long-range order. A focal point will be hybrid halide perovskites, which represent a recent breakthrough in solar energy research. These materials can efficiently convert sunlight to electricity despite displaying dynamic disorder across multiple length and time scales [1]. A microscopic understanding of this behaviour will be presented.


BIOSKETCH
Aron Walsh is Professor of Materials Theory in the Centre for Sustainable Chemical Technologies at the University of Bath. He was awarded his Ph.D in chemistry from Trinity College Dublin, completed a postdoctoral position at the National Renewable Energy Laboratory (USA), and held a Marie Curie fellowship at University College London. His research combines technique development and applications at the interface between solid-state chemistry and physics. He has published over 200 papers, with an h-index of 54. In 2015 he was awarded the EU-40 prize from the Materials Research Society for his work on the theory of solar energy materials.
Kristine Niss  
Associate Professor, “Glass and Time”, IMFUFA, Department of Science and Environment, Roskilde University

**PRESENTATION TITLE:**  
Is the glass transition universal?

**ABSTRACT**

The glass-transition phenomenon is independent of the nature of the interactions between the atoms or molecules of the liquid forming the glass. The generic character of the transition has led physicists to believe that there is a single underlying explanation of the phenomenon. Almost 20 years ago the Nobel laureate P.W. Anderson stated that understanding the glass transition is the deepest unsolved problem in solid state physics, but a satisfactory explanation is still lacking.

Understanding the glass transition implies understanding the dynamics (e.g., diffusion, vibration, relaxation) of the viscous liquid forming the glass. Experimentalists have tried to establish universal behaviors and correlations in the effort to guide the development of a theory for the glass transition. However, when more systems are studied, these results are usually found to hold only for a limited class of systems. The emerging picture is that while the glass transition can be observed in all systems independent of chemical details, there is also a myriad of specific behaviors, and it seems unlikely to capture all this in one theory. Based on this understanding, our proposal is to address the question: what is the simplest behavior is? In other words, what are the features that should be included in the “ideal gas model” of glass forming liquids?

We have studied the temperature and pressure dependence of the alpha relaxations time scale and spectral shape using a range of techniques covering dynamics from the nanosecond to the kilo-second range. Our main findings are: 1) for simple liquids there is no change in spectral shape in the entire viscous region (timescales from micro-seconds to beyond kilo-seconds) and 2) there is no temperature or pressure dependent decoupling between the relaxation times of different response functions.

**BIOSKETCH**

Kristine Niss is Associate Professor of Experimental Physics at Roskilde University, Department of Science and Environment. K. Niss is M.Sc. in Physics and Mathematics from Roskilde University 2003 and Ph.D from Laboratoire de Chimie Physique, Université Paris Sud 2007.

The group of K. Niss is part of the “Glass and Time” Center and studies the fundamental questions related to the dynamical slowing down in glass-forming systems using a variety of techniques ranging from mechanical spectroscopy to neutron spectroscopy.

The central ingredient of the work of K. Niss is tests of models and hypothesis by developing new experiments and new data analysis. Currently a focus point is developing experimental strategies for testing the isomorph theory, which has been developed in the “Glass and Time” Center.

K. Niss holds a “Sapere Aude” Starting Grant from the Danish Council for Independent Research. A main part of her project is developing a high pressure cell for simultaneous dielectric- and neutron spectroscopy in collaboration with the neutron-scattering facility ILL. K. Niss is moreover scientific responsible for the development of high precision temperature control in collaboration with the future neutron-scattering facility ESS, where K. Niss is also a member of the Scientific Advisory Board.

Sylvie Roke  
Associate Professor, École Polytechnique Fédérale de Lausanne

**PRESENTATION TITLE:**  
Aqueous nanoscopic systems

**ABSTRACT**

The molecular, structural, dynamic, and biological properties of water, aqueous systems and aqueous interfaces are essential in understanding the complexity of life, and our ability to harness examples from nature for novel (nano)technologies. Nonlinear imaging and scattering / spectroscopy methods are promising tools that can gain label free molecular-level information about aqueous systems and (nanoscopic) interfaces in three dimensions. I will introduce these methods and then consider three intriguing topics related to the nanoscale properties of water:

- Do ions influence water structure over nanoscopic length scales [1]?
- Do water molecules respond symmetrically to charge (with respect to its sign) [2]?
- Is it possible to perform label-free imaging of dynamics in living systems [3] with the aid of nonlinear optical responses from water?


**BIOSKETCH**

Sylvie Roke obtained B.Sc. and M.Sc. degrees with highest honors in chemistry (2000) and physics (2000) from Utrecht University and a Ph.D degree in natural sciences from Leiden University (2004, highest honors). In 2005 she was awarded an independent research group leader (W2) position by the Max Planck Society. In 2011 she moved to EPFL, where she holds the Jüli Jascobi chair in photomedicine. She received the Minerva Prize (2006), the Hertha Sponer Prize (2008), an ERC Starting Grant (2009), and an ERC Consolidator Grant (2014). Her research focuses on understanding aqueous systems, interfaces, soft matter, and biological systems through nanoscale imaging and spectroscopy methods.
ABSTRACT

Ionic liquids can be loosely defined as salts that are in the liquid state under ambient conditions. This arises when the constituent ions have bulky or asymmetric molecular structures so are not predisposed to crystallize. The structure and dynamics of ionic liquids cannot be explained using existing theories of electrolytes or of liquid mixtures: the extreme ion density is at odds with the dilute-limit assumption of the Debye-Hückel theory, and the existence of long-ranged Coulomb interactions prevents the use of simple mixing theories.

In my talk, I will outline some of the experimental observations that have proved hard to explain, and outline some theoretical efforts to capture the ionic liquid state. I will include some summary of my own approach, which is an experimental one: high-resolution measurements of the interaction force between atomically smooth macroscopic surfaces across ionic liquids. These experiments reveal aspects of the interfacial structure and ordering in the liquid, shear dynamic properties, and ‘anomalous’ long-range interactions more usually associated with dilute electrolytes. Overall, I will propose that ionic liquids indeed present an exciting challenge to our understanding of the liquid state.

BIOSKETCH

Susan Perkin is Associate Professor of Physical Chemistry and a Fellow of Trinity College, University of Oxford. She previously held positions at UCL in London (2007-2012) and Merton College, Oxford (2005-2008). Susan’s experimental research interests involve molecular and complex fluids at interfaces, with a recent particular focus on ionic liquids and concentrated electrolytes. In 2016 she was awarded a Starting Grant from the European Research Council and the Harrison-Meldola Memorial Prize by the Royal Society of Chemistry.
ABSTRACT
In practical applications, the surface properties of materials are often just as important as the bulk properties, if not more important. A simple, effective and versatile way of modifying surface properties is to coat it with organic macromolecules, e.g., by chemically grafting them to the substrate.

The approach to use such “polymer brushes” for surface modification has a long tradition, and I will start out with briefly reviewing the history of the field, mostly from the theorist’s perspective. I will show recent examples of applications of polymer brushes in nanocomposite design and for biomedical applications. Then I will focus on ideas to produce “smart” surfaces based on polymer-brushes, which can change their properties in response to external stimuli.

BIOSKETCH
Friederike Schmid is presently a professor in theoretical physics at the Johannes Gutenberg University Mainz in Germany. She studied physics at the universities of Heidelberg, Munich (LMU), and Mainz, and received her PhD degree in 1991 under the supervision of Prof. Kurt Binder, with a PhD thesis related to statistical physics and metallic alloys. After a postdoctoral stay at the University of Washington, Seattle, under the supervision of Prof. Michael Schick, she came back to Germany in 1994 and obtained her Habilitation in 1997. She was a junior group leader at the Max Planck Institute for Polymer Science in 1999-2000, then she became a professor at the university of Bielefeld, where she stayed until she accepted a professor position in Mainz in 2009.

Her research is devoted to the statistical thermodynamics of soft matter and complex fluids, with special focus on macromolecular systems, biologically motivated problems, flow and transport phenomena, and method development for mesoscale simulations of soft matter.

ABSTRACT
Anisotropic Janus colloids are emerging building blocks for programmable self-assembly of materials. So far, experimental studies on the self-assembly of Janus particles have focused on the behavior of small clusters formed in dilute suspensions, mainly due to the scarcity of the available colloids. Here, we demonstrate a simple, yet versatile method yielding monodisperse colloids that possess anisotropy in both shape and chemistry. We observe that these particles exhibit hierarchical self-assembly: they first form inverse cylindrical “micelles”, which subsequently stack into highly ordered lanes and ultimately form macroscopic structures. Computer simulations shine further light on the observed structures.

BIOSKETCH
Dirk Aarts is a Professor of Chemistry in the Physical and Theoretical Chemistry Laboratory at the University of Oxford and Student at Christ Church. He graduated from the University of Utrecht (Netherlands) in Chemistry (cum laude) and conducted his PhD research at the same institution, obtaining his degree in 2005 (cum laude) under the supervision of Prof. H.N.W. Lekkerkerker. He then moved to the Laboratoire de Physique Statistique, Ecole Normale Supérieure as a Marie-Curie Intra-European Fellow working with Prof. D Bonn. He started his lecturership at Oxford in 2007 and was made full professor in 2013.

He has been studying soft matter systems covering a wide range of topics revolving around phase behavior, wetting phenomena, hydrodynamic instabilities and liquid crystals. Since 2005 he has been awarded numerous prestigious prizes including the IoP Liquids and Complex Fluids Group Young Scientist Award and the Martinus van Marum Award (Royal Holland Society of Sciences). He is coordinator of a European Innovative Training Network called ‘DiStruc’.
ABSTRACT
Chemical Physics has a vast and enduring tradition in spectroscopy, atom-molecule-optics, sciences, quantum theory, surface science, soft matter, polymers, etc. On one hand, the field pushes towards understanding the fundamentals; the quantum chemistry of interactions and reactions; at the single atom/molecule level, while on the other hand the complexity of advanced materials, biosystems and networks is addressed. The challenge is to combine these two opposing directions: can one track the dynamics of molecules in action in a real-life complex (bio)environment? To this end one needs ultrasensitive single-molecule-detection, nanotechnologies to address the molecular scale and advanced fs-ps spectroscopies, all operating in harmony at environmental conditions.

Here I will present new trends to detect single molecule and proteins in their natural environment, using fluorescence, plasmonic antenna enhancement, stimulated emission and scattering methods. Next, I aim to outline schemes to exploit fs-ps spectroscopy on individual molecules. Finally, I’ll dive into nanoscale imaging of molecules using optical antennas. These trends will be illustrated with specific applications on capturing the fs-ps energy transfer in light harvesting systems.

Chiefly I hope to encourage students and young researchers to brainstorm further on the future and opportunities of chemical physics research.

BIOSKETCH
Niek van Hulst studied Astronomy and Physics, and obtained his PhD (1986) in Molecular & Laser-Physics at the University of Nijmegen (the Netherlands), on microwave-laser double resonance molecular-beam spectroscopy of molecules seen in interstellar clouds. After research periods on non-linear optics of organic materials, integrated optics, atomic force and near-field optical microscopy in 1997 he became full Professor in Applied Optics at the MESA+ Institute for NanoTechnology, University of Twente (the Netherlands) with focus on nanophotonics, optical scanning probe technology and single molecule detection.

In 2005, attracted by the Catalan open-minded, quality-based science policy, he started as ICREA Research Professor and senior group leader at IFCO—the Institute of Photonic Sciences, within The Barcelona Institute of Science & Technology.

Author of 260 refereed papers, average 44 citations/paper, h-index: 56 (WoS).

Niek van Hulst coordinates the Spanish CONSOLIDER network NanoLight.es. Also he heads the Academic Program at ICFO. Recipient of European Science Award of the Körber Foundation 2003 and City of Barcelona Prize 2010, OSAfellow, ERC Advanced Investigator Grants in 2010 and 2015.

Niek F. van Hulst
Group leader, ICFO - the Institute of Photonic Sciences, the Barcelona Institute of Science & Technology; ICREA Professor, Institució Catalana de Recerca i Estudis Avançats

PRESENTATION TITLE:
Pushing chemical physics to the nanoscale

ABSTRACT
Transient electronic and vibrational spectroscopy is traditionally and predominantly performed at the ensemble-level, largely due to the necessity of combining the response from a significant number of molecules to generate a measurable signal over any measurement noise. Although there are some recent exceptions, most notably in single molecule spectroscopy, our ability to spatially resolve electronic dynamics remains limited. Critically, however, no currently available technique is able to spatially correlate transient spectroscopic data with local molecular structure and composition, thereby considerably limiting our ability to rationalise the reasons behind any observed spatial variations in electronic dynamics.

This problem is especially acute in nanostructured electronic materials such as organic semiconductors, colloidal quantum dots and organic-inorganic metal halide perovskites. Electron microscopy or X-ray studies can easily report on the spatial inhomogeneity of thin films of these materials, yet conventional transient spectroscopies give little insight into how these variations in local structure and composition control the macroscopic electronic properties. Given the growing importance of these materials, both from the point of view of fundamental electronic properties and also for applications in next-generation photovoltaics (PVs), light emitting diodes (LEDs) and other optoelectronic devices, there is a clear and growing need for moving ultrafast electronic and vibrational spectroscopy beyond the ensemble average towards high spatial resolution. The ultimate goal of this thrust would be resolving dynamics on nanoscopic length and ultrafast time scales, simultaneously. Such capabilities will not only aid in our understanding of next generation materials, but also provide new insight into the fundamentals of light matter interactions and coherent phenomena. I will present very recent efforts and first experimental results using a novel ultrafast microspectroscopy capable of high sensitivity vibronic spectroscopy on sub-micron length scales. I will focus on early results of the transient electronic response of gold nanostructures and lead-halide perovskites.

BIOSKETCH
Philipp Kukura is a Fellow, Tutor and Associate Professor in Physical Chemistry. He received his PhD in Chemistry from the University of California, Berkeley in 2006, under the guidance of Richard Mathies in ultrafast vibrational spectroscopy. In 2006 he moved to ETH Zurich as a postdoctoral fellow joining Vahid Sandoghdar's nano-optics group. He received an EPSRC career acceleration fellowship in 2009 and moved to the Chemistry Department at the University of Oxford, establishing an independent research group. In 2011 he received the Harrison-Meldola memorial prize from the Royal Society of Chemistry, a starting investigator grant from the European Research Council (ERC) in 2013 and the Marlow award of the Royal Society of Chemistry in 2015.

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PRESENTATION TITLE:
Femtosecond time-resolved microspectroscopy

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The aim of our work is to understand the physicochemical principles that govern the highly complex process of protein aggregation. This process may lead to fatal diseases, as in the case of Alzheimer’s disease, but we can also profit from it in the form of novel nanomaterials. All-atom molecular dynamics (MD) simulations of protein aggregation in explicit solvent have been performed for over a decade, revealing valuable information about this phenomenon. However, all studies published to date suffer from at least one if not both of the following two problems.

(1) The accuracy of current all-atom force fields in modeling protein aggregation is insufficient. In a benchmark study we first compared the performance of older (e.g., OPLS) and new force fields (e.g., CHARMM22*) in their ability to model amyloid β (Aβ), an intrinsically disordered protein associated with Alzheimer’s disease, and found that the newer force fields can better reproduce the available NMR data. We then compared the same force fields for their ability to distinguish between peptides that are known to aggregate and those that do not. While the older force fields completely fail this test, the results from the new force fields are at least promising, yet not convincing. Our future work will address this problem.

(2) The second problem is that all-atom MD simulations of protein aggregation are generally performed at protein concentrations orders of magnitude higher than in vivo situations, limiting structural rearrangements between aggregate growth events. In order to overcome this limitation we currently work on the extension of the formalism of Markov state models to the study of protein aggregation. By taking into account both inter- and intra-protein details in the construction of these models, we will obtain a mechanistic understanding of the step-wise aggregation process.

BIOSKETCH
Birgit Strodel studied Chemistry at the universities of Dusseldorf (Germany) and North Carolina, Chapel Hill (USA). She received her PhD in Theoretical Chemistry from the University of Frankfurt/Main (Germany) in 2005 under the supervision of Prof. Gerhard Stock. She then spent 2006–2008 as a post-doctoral research associate at the Chemistry Department at Cambridge University (UK), working with Prof. David J. Wales. Since 2009 she heads the Computational Biochemistry Group at the Julich Research Centre (aka Forschungszentrum Jülich). In addition, she was appointed to a Professorship at Heinrich Heine University Düsseldorf in 2011. Her research primarily involves the study of protein aggregation, for which she develops and applies simulation techniques to reveal the thermodynamics and kinetics of this process.

ABSTRACT
Water is largely considered to be indispensable to life. But a molecular understanding of the role played by water in the biochemical function of proteins and DNA has long remained elusive.

Recently, tremendous developments in chemical physics research, both experimental (e.g., in femtosecond spectroscopy) and theoretical (with models and numerical simulations), have lead to a detailed description of the water hydrogen-bond network dynamics and of its changes in the presence of simple solutes. These new results now open the way to the challenging study of the water behavior in complex biochemical environments.

We will show that numerical simulations and theoretical modeling established in prior studies of smaller solutes provide a molecular description of protein and DNA hydration dynamics. In agreement with experimental observations, the hydration shell is found to be slower than bulk water, and the molecular origin of this slowdown can be now precisely identified. Whether this slowdown is rather due to the shape of the biomolecule or to its chemical exposed groups is determined unambiguously.

In a complementary study, we will focus on the influence of water on the function of proteins, to understand why the presence of water enhances the catalytic activity of enzymes. Water is usually depicted as a lubricant which facilitates the conformational transitions occurring during enzyme catalysis. Through the study of a paradigm enzyme in a nonaqueous solvent, we will assess the molecular validity of this description and suggest new routes to optimize the enzymatic catalytic activity in non-aqueous solvents.

The two studies illustrate how ideas from chemical physics can be fruitfully applied to address exciting questions arising in complex biochemical systems.

BIOSKETCH
Damien Laage received his PhD from École Normale Supérieure, Paris (ENS) with James T. Hynes. He was a postdoctoral fellow at ETH Zürich with Michele Parrinello and in 2002 he joined the ENS Chemistry Departement where he and his group study chemical reactivity and spectroscopy in solutions and biochemical environments.
**ABSTRACT**
Transition metal clusters are frequently used as model systems for low coordinated sites of extended surfaces and their study can provide valuable insights into the mechanisms of surface reactions. In many cases, however, there is still a lack of information on their structures and the relationship between structure and chemical behaviour. Using vibrational spectroscopy of gas-phase clusters one can obtain information about the clusters’ structure or the behaviour of adsorbed species. The latter provides valuable insights into the binding geometry, the activation of bonds within the ligands or reactions occurring on the clusters’ surface. Cluster size specific data can be obtained using infrared multiple photon dissociation spectroscopy. To cover the required spectral range from the far to the mid-IR, our experiments make use of IR free electron lasers. The talk will discuss exemplary studies about structures of clusters of the platinum group metals [1] and the activation of carbon dioxide by anionic cobalt [3] and rhodium clusters.


**BIOSKETCH**
André Fielicke studied Chemistry at the Humboldt University Berlin, Germany, and completed his PhD in Physical and Theoretical Chemistry in 2001. Subsequently, he worked as a postdoctoral fellow at the Infrared Free Electron Laser Facility FELIX within the FOM Institute for Plasma Physics in Nieuwegein, The Netherlands. From 2004 to 2012 he was heading a research group within the Department of Molecular Physics at the Fritz Haber Institute of the Max Planck Society in Berlin, Germany. Thereafter, he moved to the Technical University Berlin where since 2015 he has been a visiting professor at the Institute of Optics and Atomic Physics. Recently he was awarded a Heisenberg fellowship of the German Science Foundation.

His research focuses on the fundamentals of nanoscience, aiming to obtain a better understanding of the physical and chemical properties of matter at the nanoscale, mainly by experimental investigation of gas-phase clusters. His studies center upon the geometric and electronic structures and reactions of strongly bound clusters. He has contributed to the development of new experimental methods and novel experiments for the spectroscopy of such species, in particular by using infrared free electron lasers.

**ABSTRACT**
Solution-processed organic thin films and organometal halide perovskites have emerged as cost-efficient alternatives to traditional inorganic semiconductors, with promise of large-area, lightweight and flexible devices. This has led to the development of applications including photovoltaics, field-effect transistors, light-emitting diodes and bioelectronics. There is currently a knowledge gap concerning the underlying working principles, which limits the optimization of the applications. To overcome this, we investigate the light-matter interactions and transport properties in organic and hybrid semiconductors. We use a palette of experiments spanning from ultrafast spectroscopy, via Stark effect methods, terahertz techniques, photocurrent measurements, to nanoscale mobility characterization. In this talk, I will discuss what has been already achieved in the field and I will present highlights from our work about organic and perovskite-based solar cell materials and organic fluorescent biosensors. For example, the active layer of organic photovoltaic devices often consists of a conjugated polymer, blended with a fullerene derivative in a solid-state thin film. I will discuss the correlation between the phase-morphology of polymer-fullerene blends and the photogeneration/transport of free charges. Finally, I will present the main challenges that remain in the field and in particular the chemical physics questions that still need to be resolved to achieve optimal new generation semiconductors and related applications.

**BIOSKETCH**
Natalie Banerji was born and raised in Geneva (Switzerland), although she is originally Austrian. She studied Chemistry at the University of Geneva and obtained her PhD in Physical Chemistry in 2009 under the supervision of Prof. Eric Vauthey. She then moved to the University of California in Santa Barbara (USA), to work on organic solar cells during a post-doctoral stay with Nobel laureate Prof. Alan J. Heeger (2009-2011). In 2011, she was given the opportunity to start her independent research career in Switzerland at the École Polytechnique Fédérale de Lausanne (EPFL) with an Ambizione Fellowship by the Swiss National Science Foundation (SNSF). She obtained an SNSF-Professorship at the University of Fribourg (Switzerland) in 2014, and was subsequently nominated tenure Associate Professor in 2015.