"Go Physical: Symposium in Honor of 100th Anniversary of Marie Curie's Nobel Prize for International Year of Chemistry"

Special Physical Chemistry Symposium at the 2011 ACS National Meeting in Denver, CO
August 28-September 1, 2011
PI: Geraldine L. Richmond, University of Oregon

The symposium was well attended during the 4-day symposium. The invited speakers were primarily women in early career stage (~4-8 years) with a few senior women and men as invited speakers or session chairs.

Included in each day was a Poster Session for graduate students and a lunch in which the turn out was strong and the posters presented encouraged much of dialogue with the invited speakers, guests and others attending the ACS meeting and wanted to discuss the student's research and meet with the speakers.

Most all speakers and participants were very positive about the sessions and expressed that the funding to cover some expenses made it possible for them to attend the conference and the poster session luncheon.

There was a total of 51 presenters, below are the speakers and their abstracts, in order presented:

Sunday Morning Session Chair: Geri Richmond, University of Oregon

Christy L. Haynes: "Partition layer enabled surface-enhanced Raman scattering"

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In recent years, surface-enhanced Raman scattering (SERS) has emerged as a viable analytical tool. However, SERS amenable analytes are often limited to molecules with a natural affinity for noble metal substrates. The work presented herein focuses on generalizing SERS signal transduction to new classes of analytes by advancing partition layer-assisted SERS. In these experiments, partition layers are assembled on the nanostructured noble metal substrates to facilitate concentration of analytes within the zone of electromagnetic enhancement. Multiple surface science methods have been employed to characterize the assembled partition layers and how these layers change upon introduction of hydrophobic analytes. This approach has been successfully employed for sensing of mixtures of polychlorinated biphenyls and polycyclic aromatic hydrocarbons. Recent effort employs this approach for detection and discrimination of phospholipid species, moving toward measurement of cell-secreted lipid species.

John Tully: "Chemical dynamics beyond Born-Oppenheimer"

John Tully, john.tully@yale.edu, Chemistry, Yale University, New Haven, Connecticut 06520-8107, United States

Mixed quantum-classical dynamics (MQCD) has been a successful strategy for introducing quantum mechanical phenomena such as electronic transitions and tunneling, into molecular dynamics simulations. A crucial concern in MQCD is self-consistency between classical and quantum motions. The time-dependent motion of the classical variables induces quantum transitions. Quantum transitions, in turn, alter the forces that govern the motions of the classical particles. These issues have been addressed by members of my research group over many years, and will be illustrated by two examples. The first, pioneered by Sharon Hammes-Schiffer, is MQCD simulation of proton transfer in solution, where classical mechanical rate constants are often in error by orders of magnitude through neglect of tunneling and zero-point motion. The second, spearheaded by Sharani Roy and Neil Shenvi, addresses the dynamics of chemical processes at metal surfaces where nonadiabatic electron-hole pair transitions and electron transfer can dominate the transfer of energy.

Amanda J. Haes: “Nanoparticles and plasmonics”

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Precise control over the shape, shape, and local environment of nanoparticles is vital for the development of new nanotechnology applications. This is especially important in understanding how these size-dependent properties impact the detection of biological and chemical targets. In this presentation, the novel size dependent plasmonic properties of gold nanoparticles will be exploited to improve the direct and quantitative detection of disease biomarkers. Capillary electrophoresis will be used to reduce the amount of biological sample required per assay. Detection sensitivity and specificity will be shown to depend on the nanoparticle size and surface chemistry homogeneity. This detection approach offers new and promising methods for the rapid, selective, and sensitive detection of biomarkers.

Christy Landes: “Wavelet shrinkage to resolve single molecule FRET structural landscape of the isolated ligand binding domain of the AMPA receptor”

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Single molecule fluorescence resonance energy transfer (smFRET) was used to examine the conformations explored by the agonist binding domain of the ¬⋏-amino-3-hydroxy-5-methyl-4-isoxazole propionate receptor. It was found that the glutamate-bound form explores a wide range of conformations. The distribution of conformations in the raw data was so wide it was not possible to extract conformational details. By employing a model-free data analysis technique called wavelet shrinkage, it was determined that each protein form comprised multi-state, sequential equilibria. The results illustrate that the extent of activation is dependent not on a rigid closed cleft, but instead on the probability that a given subunit will occupy a closed cleft conformation, which in turn is determined by the range of states that the protein explores. Also, the results emphasize both the need for and the utility of advanced data processing techniques to quantify structure and dynamics in heterogeneous systems.

Elsa C.Y. Yan: “Chiral sum frequency generation spectroscopy for characterizing protein secondary structures at interfaces”

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Characterization of protein secondary structures at interfaces is important in biological and bioengineering sciences, yet remains technically challenging. Here, we used chiral sum frequency generation (SFG) spectroscopy to establish a set of chiral vibrational optical markers for identifying protein secondary structures at interfaces, similar to the use of circular dichroism for characterizing secondary structures in bulk solution. Using chiral SFG, we detected characteristic chiral N-H stretch and amide I vibrational signatures of peptide backbones unique to random-coil, alpha-helix, and beta-sheet at interfaces. Using these chiral vibrational signatures, we monitored human islet amyloid polypeptide *in situ* and in real time as it misfolds from random coils to alpha-helices and then beta-sheets, upon interaction with a lipid-water interface. Our findings show that chiral SFG spectroscopy is a powerful tool to follow changes in protein conformations at interfaces and identify interfacial protein secondary structures that are hard to resolve using conventional techniques.

Jennifer A. Hollingsworth: "Nanocrystal quantum dot architectures and assemblies for light emission applications"

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Due to their characteristic bright and stable photoluminescence, semiconductor nanocrystal quantum dots (NQDs) have attracted much interest as efficient light emitters. Despite these enabling traits, however, NQD optical properties are frustratingly sensitive to their chemical environment, exhibit fluorescence intermittency ("blinking"), and are susceptible to Auger recombination, an efficient nonradiative decay process. Here, I review our work on the development of a new class of NQD that we have called "giant" NQDs, due to their relatively thick inorganic shell. We demonstrate unprecedented non-blinking behavior and suppressed Auger recombination toward realizing applications in single-particle tracking and efficient solid-state lighting. Key advances were achieved by tuning NQD physical and electronic structure, and the underlying principles are being applied to multiple semiconductor compositions. Lastly, in addition to realizing novel light-emission properties by refining nanoscale architectures at the single-NQD level, we also investigate collective properties achieved by assembling our core/shell NQDs into larger scale arrays.

Sunday Afternoon Session Chair: Nancy Levinger, Colorado State University

Valeria Molinero: "Crystallization of water: From bulk to the nanoscale"

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One of water's unsolved puzzles is what determines the lowest temperature at which liquid water and aqueous solutions can be cooled before freezing to ice. Knowledge of the freezing temperature of water is crucial in areas as diverse as climate modeling, the design of new materials and biopreservation. Water crystallization requires the spontaneous formation of ice nuclei within the liquid. The increase of ice nucleation rates as water is supercooled correlates with a dramatic increase in the heat capacity and compressibility of supercooled water, suggesting that a structural transformation occurring within the liquid phase may control the rate of nucleation of ice. We use molecular simulations to elucidate the mechanism of water freezing and its relation to the thermodynamics and structure of supercooled water. We show that the kinetics of water freezing is controlled by a structural transformation in supercooled liquid water that blurs the boundary between the liquid and crystal states. We will discuss whether this implies the end of the liquid state, what confinement of water in nanopores can teach us about the nature of that transformation and how the structures formed and nature of phase coexistence are radically changed when water is confined in nanoscopic volumes.

Irina Paci: "Theoretical investigations of surface self-assembled structures: The case of azobenzene switching"

Irina Paci, ipaci@uvic.ca, Christopher Chapman. Department of Chemistry, University of Victoria, Victoria, Canada

One of the main objectives of nanoscale research is the bottom-up creation of devices with complex

functions. When the device is supported on a solid surface, the impact of the substrate has to be considered in designing the self-assembly process. Theoretical investigations of surface adsorption, self-assembly, and the properties of the resulting materials are challenging. This is because quantum mechanical information about the molecules, the surface, and their interactions must ultimately be incorporated in bulk simulations. This talk will describe some of our group's efforts in advancing the understanding of the field-induced switching in mixed alkylthiol/azobenzene monolayers. The results of our sequential multiple-scale approach to examine the field and density dependence of the switching process will be discussed.

Richard P. Van Duyne: “Recent advances in molecular plasmonics”

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The detailed understanding of the interactions between adsorbed molecules and plasmonic nanostructures (i.e., molecular plasmonics) is having a significant impact in many areas of plasmonics research including surface-enhanced Raman spectroscopy (SERS), new materials, optical microscopy, localized surface plasmon resonance (LSPR) spectroscopy for chemical and biological sensing, and nanolithography.

This lecture will focus on recent developments from the outstanding women scientists in the Van Group in three areas: single nanoparticle SERS (SPSERS) and single molecule SERS (SMSERS); high resolution transmission electron microscopy (HRTEM) spatially correlated with SPSERS and SMSERS; and wide-field LSPR imaging for biosensing and the spectroscopic characterization of nanoparticles in motion.

Christine M. Aikens: “Theoretical studies of noble metal nanoparticle physical properties”

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Monolayer-protected gold and silver nanoparticles have a unique surface structure that affects their physical properties. Density functional theory calculations are employed to examine the electronic structure of these systems. The superatom model can be used to explain optical absorption and EPR properties of nanoparticles such as $Au_{25}(SR)_{18}^{-1,0}$. In addition, this model aids in the understanding of chiroptical properties. Excitations between superatom orbitals are responsible for the low-energy metal-metal transitions observed in absorption and circular dichroism spectra. Theory-experiment agreement can be used to predict the structures of nanoparticles for which no crystal structure is available.

Sophia C Hayes: “Analysis of the excited-state absorption spectral bandshape of oligofluorenes”

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Ultrafast transient absorption spectra of two oligofluorene derivatives in dilute solution will be presented, These spectra display a photoinduced absorption band with clear vibronic structure, which is analyzed rigorously using the time-dependent formalism of absorption to extract the principal excited-state vibrational normal-mode frequencies that couple to the electronic transition, the configurational displacement of the higher-lying excited state, and the reorganization energies. The excited-state spectrum is modeled using two totally symmetric vibrational modes with low and high frequencies. We find that the reorganization energy of the ground-state absorption is insensitive to the oligomer length, while that of the excited-state absorption evolves significantly between the oligofluorene dimer and trimer. The absorption spectra are assigned to a transition from the $1B_u$ excited state to a higher-lying mA_g state. These results and analysis permit profound understanding of the nature of excited-state absorption in π-conjugated polymers, which are the subject of general interest as organic semiconductors in the solid state.

Julia Laskin: “Preparation of novel materials using soft- and reactive landing of mass-selected ions”

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Ion-surface collisions are utilized in materials science, mass spectrometry, imaging and spectroscopy. Our research is focused on obtaining a fundamental understanding of interactions of hyperthermal (1-100 eV) complex ions with organic surfaces. Soft landing of ions is defined as intact deposition on surfaces with or without charge retention. Alternatively, ion-surface collision may induce reactive deposition of the precursor ion or its fragments on the surface. This process is called reactive landing. Preparatory mass spectrometry utilizes soft-landing and reactive landing of complex ions on surfaces for highly specific preparation of novel materials. Deposition of mass-selected ions on surfaces is accompanied by a number of processes including charge reduction, neutralization, covalent and non-covalent binding, and thermal desorption of ions and molecules from the substrate. Factors that affect the competition between these processes will be discussed. Several examples of controlled deposition of complex ions on self-assembled monolayer surfaces demonstrating the utility of preparatory mass spectrometry for highly-selective preparation of biological and catalytic surfaces will be discussed.

Monday Morning Session Chair: Branka Ladanyi, Colorado State University-Fort Collins

Marcia Levitus: “Fluorescence fluctuation spectroscopy: The study of kinetic processes in equilibrium conditions”

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Recent developments in single molecule detection made it possible for the first time to study dynamic processes at equilibrium. These techniques have had the most impact in the investigation of the conformational dynamics of biopolymers, where they are traditionally labeled with fluorescent probes that are sensitive to the conformational state of the biomolecule.

When one or a few molecules are observed at the time, fluctuations in the conformational state of the biopolymer produce fluctuations in fluorescence intensity that can be detected and analyzed. The analysis of these fluctuations allows the kinetic investigation of reactions at equilibrium, without the need of applying external perturbations such as those used in common relaxation methods.

In this talk, I will provide an overview of the capabilities of fluctuation spectroscopy methods to investigate conformational dynamics in biopolymers, and discuss our recent research on the application of fluctuation techniques to investigate dynamics in protein-DNA complexes.

George C Schatz: “DNA in nucleosomes: Mechanical properties and TT photodimerization”

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This talk focuses on the properties of DNA when wrapped around the histone proteins in nucleosomes. There has been an important realization in the last ten years that there are important propensities which govern the base-pair compositions that favor nucleosome location, with AA, AT or TA often found whenever the minor groove points inward. In this talk we describe the use of molecular mechanics and dynamics to study the mechanical stability of DNA, and why certain base-pair compositions are commonly found in nucleosomes. We also show how TT photodimerization depends on base-pair composition, and how this is connected to nucleosome structure.

Serena DeBeer: "Probing biological catalysis using K-Beta X-ray emission spectroscopy"

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The development of K-Beta X-ray emission spectroscopy as a novel probe of metal spin and oxidation state, as well as metal-ligand interactions is described. Initial studies on model complexes, highlight the information content of the valence to core spectra and show the sensitivity of these spectra to the nature (ㅇ -donating, ㅈ ㅈ -donating, and ㅈ ㅈ -accepting) and identity of the bound ligands. A close correlation of experimental data to theory allows for a deeper understanding of spectral features. The potential of XES for characterizing intermediate species in non-heme iron enzymes is highlighted. Recent applications to nitrogenase and methane monooxygenase are discussed.

Nien-Hui Ge: "Probing peptide structure and dynamics using multidimensional infrared spectroscopy and isotopic substitution"

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Femtosecond multidimensional IR spectroscopy is a powerful technique that can provide new insights into chemical and biological processes. In this talk I will present an overview of our recent work on using this technique and isotope labeling to study the structures and dynamics of peptides. The cross-peaks in the amide-I and II regions reveal couplings between these modes that are sensitive to the peptide structure. Isotope substitution enables us to probe vibrational couplings between structural units in a site-specific manner. Moreover, it reports structural dynamics associated with local environment fluctuations. Results will be presented on oligopeptides with different secondary structures and supercoiled protein motifs. The experimental data are compared with computational results obtained from molecular dynamics simulations and quantum-chemical calculations.

Laura J. Kaufman: "Delineating time and length scales of heterogeneity in supercooled liquids"

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Supercooled liquids display behaviors consistent with the presence of heterogeneous dynamics. We investigate the length scales over which such heterogeneities exist and the time scales over which they persist using single molecule (SM) fluorescence microscopy. To investigate whether probe properties affect breadth of heterogeneity reported in a given host system, four different probes are studied in supercooled glycerol. Across all probes, rotational relaxation times of probe molecules are found to be log-normally distributed. No significant change in relaxation time distribution as a function of temperature is evident for a given probe. However, across probes, probe rotational relaxation time is correlated with breadth of heterogeneous dynamics reported. Taken together with complementary measurements indicating that such molecules undergo changes in their dynamics on the shortest time scales probed, these experiments establish a lower bound on the size and an upper bound on the persistence time of heterogeneity in supercooled glycerol.

Judy E. Kim: "Role of protein environment on multi-step electron transfer reactions"

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Long-range electron transfer (ET) reactions in biological systems often utilize amino acid radicals as redox-active intermediates. These intermediates allow ET to occur over long distances in a manner more efficient than the analogous single-step process. Our group recently reported a photoinduced ET reaction from the native tryptophan residue to the metal center in a blue copper protein, azurin. This ET process is followed by deprotonation to form a stable neutral tryptophan radical. Here, we present new spectroscopic findings for wild-type azurin in which production of the neutral radical is quenched because of proton-coupled electron transfer (PCET) from a nearby tyrosine residue. This multi-step ET reaction results in charge separation over ~20 Å, and occurs rapidly because of the optimized position and hydrogen-bonding of the tyrosine residue. Knowledge of the role of the protein environment on PCET efficiency will facilitate the incorporation of radical intermediates into ET pathways, and potentially inspire new biomimetic materials.

Christine K. Payne: "Imaging chemical reactions inside living cells: Two-color single particle tracking of the enzymatic degradation of low-density lipoprotein (LDL)"

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Cells control many intracellular reactions through localization of substrates and enzymes within distinct vesicles. These vesicles are actively transported through the cell, thereby overcoming the barrier of limited diffusion within the crowded environment of the cytosol. The goal of research in the Payne Lab is to understand the mechanisms of intracellular reactions in light of the additional complexity associated with vesicle transport. Two-color single particle tracking was used to probe the intracellular degradation of LDL in living cells. Individual LDL particles were labeled with multiple fluorophores resulting in a quenched fluorescent signal that increased intensity upon degradation. The transient colocalization of LDL with early and late endosomes, fluorescently labeled with variants of GFP, was imaged while simultaneously measuring the intensity of the LDL particle as an indicator of degradation. These experiments show that degradation occurs in the late endosome and characterize the endosomal interactions necessary for degradation to occur.

Monday Afternoon Session Chair: Mary Jane Shultz, Tufts University

Mostafa El-Sayed: "Some exciting properties of gold nanoparticles with applications in fields ranging from energy to medicine"

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A summary of metallic gold properties when confined to the nanoscale will be summarized. The new optical (plasmonic) properties of gold nanoparticles in enhancing light scattering processes are used in cancer detection and in imaging the different phases of living and dying cells. Their strong absorption property and rapid conversion into heat is used in the photo-thermal therapy of cancer. Their small size enabled us to conjugate them to the nuclei of cancer cells which stopped cell diviision leading to their death. Their ability in inhancing the rate of light absorption of nearby molecules made it possible for us to greatly enhance the photocurrent produced from the conversion of solar energy by the other photo-synthetic system in nature, bacterio-rhodopsin.

Rachel W. Martin: “Instrumentation and methods development for switched-angle spinning NMR of oriented membrane systems”

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Variable Angle Spinning (VAS) and Switched Angle Spinning (SAS) provide isotropic-anisotropic correlations. Recent work in our group has focused on optimizing SAS hardware and methods for measuring scaled dipolar couplings in oriented membrane systems and other mobile solids. We have developed a 500 MHz ^{1}H-^{13}C double-resonance SAS probe optimized for oriented membrane systems. It incorporates a transverse, high-homogeneity radiofrequency coil that moves with the sample in order to maximize the filling factor. The coil is connected to the static part of the probe using capacitive coupling, eliminating sliding or flexible contacts. Pneumatic switching of the spinning angle eliminates magnetic motors and allows reproducible switching on a timescale of about 15 ms.

In systems where the dipolar couplings are partially averaged by molecular motion, cross-polarization is modulated by sample spinning. The cross-polariation efficiency in VAS and SAS experiments on mobile samples is therefore strongly dependent on the spinning angle. We describe simulations and experimental measurements of these effects over a range of spinning angles from 0 to 90 degrees. Perspectives for future extensions to more dimensions and increasingly complicated systems will also be discussed.

Wendy J Shaw: “Enhancing homogeneous hydrogen production and oxidation catalysts with a designed outer coordination sphere”

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We are attaching an outer coordination sphere (OCS) to redox active catalysts which oxidize and produce H_2, mimicking hydrogenase which efficiently interconverts H^+ and H_2. Initial work has focused on incorporating small peptides around the active site of the $Ni(P_2^{R}N_2^{R'})_2$ hydrogen production/oxidation catalysts to explore how the local environment around the active site can influence catalytic rates. We have found that the peptide catalysts retain the activity of the parent catalyst, while demonstrating that regions remote from the active site do modulate activity. Currently, incorporation of larger peptides is being pursued with a combined computational and experimental approach to allow the investigation of three features of the OCS: precise control of the environment around the active site, the incorporation and evaluation of proton channels and the role of controlled dynamics. Structural data of the catalysts, activity and the role of the OCS in enzymes and homogeneous catalysts will be discussed.

Ruxandra I. Dima: “Large-scale molecular simulations of dynamics in mechanical proteins”

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Dynamic force spectroscopy provides unique opportunities for probing the free energy landscape of biomolecules. However, even if it provides information on the chain extension, it cannot supply full details of the populated structures. This is especially true in the case of multi-domain proteins for which the complexity of the fold translates into many unfolding scenarios. I will present our investigations into the role of protein-protein interactions during biomechanical unfolding reactions of multi-domain protein complexes covering various cellular functions from fusion to cytoskeletal support in experimental time . To obtain the force extension curves using experimental pulling speeds, we employed a coarse-grained minimalist model (SOP) of proteins. I will discuss the signature of the protein-protein interactions as a function of the applied vector force, and the connection between the shape of the force peaks and the degree of cooperativity in the protein complex.

Jennifer S. Martinez: “Characterization and application of small-molecule- and DNA-templated gold and silver fluorescent nanoclusters”

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Fluorescent metal nanoclusters (<1 nm) are collections of several to tens of atoms of gold or silver. While for gold nanoclusters, the fluorescence emission is thought to scale as a function of the number of atoms within the cluster, for silver nanoclusters, the relation of atom number to fluorescence emission is less clear, as is the nature of the complex/cluster. Nevertheless, “fluorescent metal nanoclusters” are gaining much interest because of their desirable photophysical properties, smaller size than quantum dots, and inherent biocompatibility. As a compliment to quantum dots and molecular fluorophores, fluorescent metal nanoclusters have been produced using templates of dendrimers and polymers, small molecular ligands, or within biological materials of interest, such as DNA. We will discuss the palette of different fluorescent nanoclusters, their synthesis and characterization, and application for biological sensing and imaging.

Caroline Ajo-Franklin: “Creating electrical interfaces between biological and inorganic materials”

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Our laboratory is interested in manipulating processes at the interface between living cells and inorganic materials to both better understand analogous natural systems and for a wide range of applications. In my talk, I will discuss our efforts to engineer bi-directional electronic communication between living cells and non-living systems. We have recently demonstrated that by transplanting a synthetic gene into the model organism *Escherichia coli* we can confer upon these cells the ability to reduce both metal ions and solid metal oxides. This work provides the first example of a predetermined, molecularly-defined route for electronic communication between living cells to inorganic materials. Ultimately we seek to exert such control over processes at the cellular-inorganic surface that our engineered cells become a new generation of self-replicating, programmable 'living materials.'

Tuesday Morning Session Chair: Veronica Vaida, University of Colorado

Richard N. Zare: “My life with LIF”

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I will present a personal account of the birth of laser-induced fluorescence (LIF) and how this technique has grown in importance over the years. I wish to preface this talk by a few remarks on the importance of creating and maintaining a family friendly department as I step down from being Chair of the Stanford Chemistry Department for the past six years

Barbara Ervens: “Effects of chemical processes on clouds and particulate matter in the troposphere”

Barbara Ervens, barbara.ervens@noaa.gov, Chemical Sciences Division, NOAA/ESRL, Boulder, CO 80305, United States and Cooperative Institute for Research in Environmental Sciences, University of Colorado, Boulder, CO 80305, United States

Atmospheric chemistry deals with the transformation of species in gas and condensed phases whereas the latter comprises aerosol particles or cloud and fog droplets. In each of these phases unique chemical processes can occur that modify their composition and the overall chemical budgets in the atmosphere. While sulfur oxidation in clouds leading to 'acid rain' is probably one of the best-understood aqueous phase processes, a plethora of organic molecules from various emission sources can also react in cloud droplets and small amounts of aerosol water modifying the mass and properties of cloud condensation nuclei.

Numerical models studies are used to test our understanding of the underlying processes and parameters that have been derived based on laboratory studies. I will show examples how such aerosol and cloud chemistry models are developed and applied to observations in the atmosphere.

V. Faye McNeill: “Atmospheric aerosols: At the interface between chemistry and climate”

V. Faye McNeill, vfm2103@columbia.edu, Chemical Engineering, Columbia University, New York, New York 10027, United States

The chemistry of atmospheric aerosols largely determines their direct and indirect effects on climate. I will present results of our recent laboratory studies showing that particle-phase chemical reactions between organics and inorganic salts can lead to secondary products which absorb light in the UV and visible, thus changing the optical properties of the particle. We also have studied the sources and properties of surface-active organic species in aerosols. Organic films at the gas-aerosol interface can reduce aerosol surface tension, potentially enhancing the ability of small particles to nucleate cloud droplets (CCN activity). Our work has shown that uptake of methylglyoxal, acetaldehyde, and formaldehyde from the gas phase driven by aqueous-phase oligomerization chemistry is a potentially significant source of surface-active organic material in aerosols. Aerosol chamber studies of the CCN activity of particles exposed to gas-phase surfactants will be presented.

Alla Zelenyuk: “Multidimensional characterization of individual aerosol particles”

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Aerosols play an important role in many areas in a manner that depends on multiple physical and chemical properties, many of which are strongly coupled. The size, internal composition, density, shape, morphology, fractal dimension, hygroscopicity, index of refraction, activity as cloud condensation nuclei and ice nuclei, and other individual particles attributes all play a role. Traditional particle characterization approaches rely on separate parallel measurements that average over an ensemble of particles of different sizes and/or compositions and later attempt to draw correlations between all observables. In this approach, differences between individual particle properties and even between particles and bulk are often missed. We will present new approaches to measure simultaneously *in-situ* and in real-time, several of the attributes for individual particles using single particle mass spectrometer, SPLAT II. We also discuss novel approaches developed for classification, visualization and mining of large datasets produced by the multidimensional single particle characterization.

Juliane L Fry: “Nighttime formation and processing of atmospheric organic aerosol by nitrate radical”

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The formation of atmospheric aerosol from oxidation of volatile organic compounds remains very poorly characterized, and represents a major anthropogenic influence on atmospheric chemistry. At night, concentrations of nitrate (NO3) radical can build up in polluted regions and provide an efficient pathway to aerosol formation. We present results of laboratory environmental chamber measurements, regional atmospheric chemistry model calculations, and field measurements to constrain the role of nitrate in atmospheric aerosol formation and degradation.

Susanna L. Widicus Weaver: “Spectroscopy of organic radicals and ions in the \'THz-Gap\"

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Transient species such as radicals and ions are common reaction intermediates and play fundamental roles in all areas of chemistry. Despite the importance of transient species in chemical mechanisms, the intramolecular interactions that dictate their reactions are not fully-understood. Such interactions lead to distinct spectral signatures, and these "fingerprints" can only be accessed through high-resolution gas-phase spectroscopy. The strongest spectral signatures for many transient molecules occur in the terahertz (THz) range, but THz spectrometer sensitivity has lagged behind techniques at shorter and longer wavelengths. We are therefore combining novel production techniques with development of high-sensitivity THz instruments to examine the spectra, structure, internal motion, and reaction dynamics of transient molecules, with an emphasis on organic radicals and ions that are important in interstellar chemistry. I will overview the challenges of THz transient molecule spectroscopy, report on progress toward high-sensitivity THz spectrometers, and present preliminary results for our initial molecular targets.

Barbara D'Anna: “Fine aerosol characterization and source apportionment in urban environments: Marseille and Grenoble (France)”

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This study presents comprehensive results of the FORMES program based on two field campaigns: one in a coastal Mediterranean city (Marseille, France) during summer 2008, the other in Grenoble, located in an Alpine valley, during winter 2009.

On line instruments (C-TOF-AMS, HS-PTR-MS, SMPS, and VHTDMA, aethalometer) were employed to investigate fine particles (PM2.5) and VOCs together with filter-based measurements (for EC and OC, ionic species, metals).

Various source apportionment methods as Positive Matrix Factorization, Chemical Mass Balance and aerthalometer model (only for Grenoble) were undertaken to evaluate the organic contribution and sources of the fine aerosol. In Grenoble, residential wood burning emissions accounted for approximately 40-50% of fine carbonaceous aerosols. Such results underline the significant impact potentially played by residential wood burning emissions on particulate air pollution in large European urban centres.

While in summertime in Marseille four major factors have been identified; the predominant factor is highly oxygenated (OOAI and OOAII type). A minor and not non-defined 4th factor called 'industrial' is found and perfectly correlates with “hot spot of PAHs” (not related to traffic emissions) which seems to related to” industrial organic source” (refinery). An excellent agreement found between PMF2/AMS analysis and CMB model.

Source apportionment methods and results from the two studies will be compared and discussed.

Tuesday Afternoon Session Chair: Vickie Grassian, University of Iowa

W. Carl Lineberger: “Anion photoelectron spectroscopy: From radicals to the reaction co-ordinate”

W. Carl Lineberger, WCL@JILA.Colorado.edu, Department of Chemistry and JILA, University of Colorado, Boulder, CO 80309-0440, United States

Anion photoelectron spectroscopy has proven to be a remarkably powerful tool to obtain fundamental thermochemical information and structural information for stable and transient species. Extension of the methodology to time-resolved anion photoelectron spectroscopy enables following reactive events along a reaction coordinate. I review the methodology and discuss examples that illustrate the possibilities: peroxyl radicals, oxyallyl diradical, and solvent-induced long range electron transfer between atoms.

Gordana Dukovic: “Electron transfer in nanocrystal-enzyme complexes for photochemical H_2 generation”

*Molly B. Beernink[1], Katherine A. Brown[2], Paul W. King[2], **Gordana Dukovic**[1], gordana.dukovic@colorado.edu. (1) Department of Chemistry and Biochemistry, University of Colorado Boulder, Boulder, CO 80309, United States, (2) Biosciences Center, National Renewable Energy Laboratory, Golden, CO 80401, United States*

Combing the superb optical properties of semiconductor nanocrystals with the efficient, selective, and robust catalysis afforded by enzymes, we have developed nanocrystal-hydrogenase complexes that generate H_2 under visible illumination. In these systems, photogenerated electrons transfer from the nanocrystal to the enzyme, which then catalyzes the reduction of H^+ to H_2. In this presentation, our efforts to map out the rates and efficiencies of transfer of photogenerated electrons by ultrafast transient absorption spectroscopy will be described. We expect this process to be the rate limiting step that determines the overall efficiency of H_2 generation. The results of the spectroscopic studies will be correlated with measurements of overall quantum efficiency of H_2 production.

R. Lee M. Penn: “In situ characterization of nanoparticle aggregation”

Nathan D. Burrows, Tram Anh Do, T. Ryan Knutson, Kairat Sabyrov, Jennifer A. Soltis, Amanda M. Stemig, Virany M. Yuwono, R. Lee M. Penn, rleepenn@umn.edu. Department of Chemistry, University of Minnesota - Twin Cities, Minneapolis, MN 55455, United States

A major research focus in the Penn group is pairing careful solid-state characterization with quantitative kinetics of reaction, nanoparticle growth, and phase transformations. Particle surfaces play important roles in natural and engineered environmental systems, and aggregation state can dramatically change accessible surface area. In addition, aggregation state is dynamic, and rates are sensitive to the dynamics

of aggregation. Transitions between different states of aggregation (e.g., ranging from single-phase fractal aggregates to mesocrystals composed of oriented primary nanocrystals to heterogeneous aggregates of two or more phases) can be directly linked to evolving kinetics of redox reactions and phase transformation.

Elizabeth A Raymond: “SHG studies of polycyclic aromatic hydrocarbons (PAH\'s) at the air/water and hexane/water interfaces”

Elizabeth A Raymond, elizabeth.raymond@wwu.edu, Everett D. Jackson, Jennifer L. McCarville. Department of Chemistry, Western Washington University, Bellingham, WA 98225, United States

Polycyclic aromatic hydrocarbons (PAH's) are produced via a number of anthropogenic sources, including incomplete combustion, as well as naturally occurring in crude oil. A large number of these compounds have been shown to be toxic and/or carcinogenic to living organisms. While the sources and environmental concentrations of these compounds have been extensively studied, much less is understood about their behavior at aqueous solution interfaces with either air or oil. The surface specific technique, second harmonic generation (SHG), in conjunction with interfacial tension measurements has been used to understand the adsorption dynamics, equilibrium surface concentrations, and surface orientations of several PAH molecules such as dibenzofuran, anthracene, and several of its acid functionalized erivatives at both the air/water and oil/water interfaces.

Amber T Krummel: “Exploring lipid-induced conformational dynamics of surfactin”

Amber T Krummel, amber.krummel@colostate.edu, Department of Chemistry, Colorado State University, Fort Collins, CO 80523, United States

Surfactin is a small, cyclic lipopeptide that is self-generated and secreted by the bacteria *Bacillus subtilis*. Surfactin has been shown to induce biofilm growth by forming ion-conducting pores which allow the leakage of potassium ions required for signaling purposes. Interestingly, Surfactin also has hemolytic, antiviral, antibacterial, and antitumor properties—it is not yet established whether the same mechanism is involved in all of these activities. We are exploring the conformational dynamics of Surfactin using two-dimensional infrared spectroscopy and monitoring spectral shifts in the Amide I vibrational mode. A tunable bicelle system is used to model natural lipid membranes in these experiments. Upon interacting with the bicelle, the lineshapes and center frequencies of the Surfactin Amide-I vibrations are strongly modulated. We will present our early explorations of these lipid-induced conformation changes exhibited by Surfactin.

Etsuko Fujita: “Carbon dioxide reduction using transition-metal complexes”

Etsuko Fujita, fujita@bnl.gov, Carol Creutz. Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973-5000, United States

We have been investigating the thermodynamics and kinetics of CO_2 binding and reduction using transition-metal complexes for over two decades. We believe the solar generation of fuels (stored in the form of chemical bonds such as CO, formate, methanol, etc. from CO_2) as an essential solution for CO_2 utilization, yet sunlight-driven CO_2 reduction to C1 fuels remains a formidable problem. We will identify several barriers for the efficient production of solar fuels and hope to stimulate research in this field. Selective topics of our recent investigations will also be presented.

Wednesday Morning Session Chair: Allison A. Campbell, Pacific Northwest National Laboratory

George W Flynn: "Probing graphene chemistry and electronic structure in two dimensions: A sub-nanometer view"

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We have used Scanning Tunneling Microscopy (STM) to investigate the structure and electronic properties of single sheets of graphite (graphene) on both insulating and metallic surfaces. STM reveals variations in electron tunneling images for these samples, when mounted on silicon dioxide and mica substrates, that differ markedly from those of multi-layer graphite. Graphene grown by CVD techniques on copper and cobalt shows different degrees of electronic coupling to the underlying substrate. These kinds of investigations have been extended to the study of surface chemical reactions where Scanning Probe Microscopy is used as a "camera" to observe defect growth in single and multiple graphene sheets exposed to oxygen. Incorporation of N-atoms into graphene's honeycomb structure has been observed for samples grown on copper during CVD exposure to ethylene and ammonia. Chemistry on these model surfaces determines the nanoscale properties of graphene and its potential use in solar energy applications

Delia J Milliron: "Near infrared electrochromism of doped colloidal nanocrystals"

Delia J Milliron, dmilliron@lbl.gov, Guillermo Garcia, Anna Llordes, Evan Runnerstrom, Raffaella Buonsanti, Andre Anders, Rueben J Mendelsberg, Thomas J Richardson. Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States

Electronically doped metal oxide nanocrystals, such as indium tin oxide (ITO) and aluminum-doped zinc oxide (AZO) exhibit surface plasmon absorption in the near infrared (NIR). In addition, chemical strategies have been developed for achieving conducting networks of nanocrystals that were initially passivated by insulating hydrocarbon ligands. Starting with well-controlled colloidal synthesis, we achieve nanoporous films with variable feature size and doping level.

We are investigating these films' potential as electrochromic coatings that selectively modulate NIR transmittance while maintaining near unity transparency for visible light, which is of keen interest for energy efficient windows. Positioning a nanocrystal film as the working electrode in an electrochemical cell, the carrier population - and thus the NIR transmittance - responds dynamically to an applied bias. Work is underway to correlate the dynamic spectral response with doping and nanocrystal size variations and, eventually, to optimize the dynamic range of transmittance for solar NIR radiation.

Amity Andersen: "Simulation and modeling studies in catalysis: Applications to biomass fuel and fine chemicals synthesis"

Amity Andersen, amity.andersen@pnl.gov, EMSL, Pacific Northwest National Laboratory, Richland, Washington 99352, United States

This talk highlights recent theoretical work on catalysis topics pertinent to efforts toward environmentally-friendly and sustainable technologies in the replacement of fossil fuels and in the production of industrial chemicals. In the first part, I will discuss recent work on catalysts that convert biomass-derived syn-gas to fuel such as alkali-promoted molybdenum disulfide, a promising catalyst selective for mixed alcohols. In the second part, I will discuss work on the *para*-selectivity nitration of mono-substituted aromatics in zeolites such as H^+-beta. The *para* isomer of mono-substituted aromatics is often the more desirable isomer for fine chemical synthesis, and solid acid catalysts such as beta zeolite demonstrate notably higher para-selectivity, which produce less harmful waste products than the traditional nitric-acid/sulfuric-acid solution. DFT calculations are used to explore potential reaction paths

and show that the original mechanism, based solely on experimental liquid and solid-state NMR data, may be disputed.

Laura Smilowitz: “Thermal explosions: Sub-sonic deflagration in high explosives”

Laura Smilowitz, smilo@lanl.gov, Bryan Henson. Physical Chemistry and Applied Spectroscopy, Los Alamos National Lab, Los Alamos, NM 87545, United States

Our team has been studying the response of high explosives to abnormal thermal scenarios with the ultimate goal of predicting the reaction violence of the plastic bonded explosive PBX9501 to such an event. The primary energetic material in PBX9501 is the organic crystal HMX, an important military explosive and rocket propellant ingredient. HMX has proven to provide a rich physical chemistry toolbox. Our most recent advances in understanding thermal explosions are based on the ability to perform high energy radiography (such as proton and x-ray) of thermal explosion events. Radiography of super-sonic detonation events in these materials has been informing the community for over 50 years, however radiography of sub-sonic deflagration has only recently been enabled by advances in our understanding and ability to control thermal explosion events. I will show images of this density evolution and describe our current state of understanding and predictability for thermal explosion events.

Lydia Finney: “Advancing the frontiers of bioinorganic chemistry through X-ray fluorescence imaging”

Lydia Finney, lfinney@aps.anl.gov, X-ray Science and Biosciences Divisions, Advanced Photon Source, Argonne National Laboratory, Lemont, Illinois 60439, United States

Our understanding of the cell biology of metals is at a point of rapid expansion, and x-ray fluorescence imaging is a key technology enabling this growth. Direct visualization of endogenous metals is revealing unique insights into their cellular dynamics, as illustrated by our work on angiogenesis, as well as the work of many others. We are pioneering new capabilities, which will work together in a complementary way to further accelerate life science. These developments, including the ability to visualize metals in biological specimens with far greater speed and to place their dynamics into the context of protein pathways, promise to bring new vision to our understanding of life.

Dana M. Dattelbaum: “Shock-driven chemical reactivity and its implications”

Dana M. Dattelbaum, danadat@lanl.gov, Stephen A. Sheffield, Virginia W. Manner, Raja S. Chellappa, Raymond P. Engelke. Department of Shock and Detonation Physics, Los Alamos National Laboratory, Los Alamos, NM 87545, United States

Interrogating chemical reactions behind a shock front is immensely difficult, and as a result, the details of shock-induced chemistry remain poorly understood. Questions regarding the thresholds for incipient reaction, the nature of first and subsequent reaction steps, and the influence of shock input conditions on reaction kinetics remain to be answered. Evidence of reaction can be discerned from discontinuities in the mechanical variables associated with a change in density along the reaction coordinate. Here, we have applied in-situ electromagnetic gauging at multiple Lagrangian positions under shock compression to elucidate shock-induced reactions. We have investigated shock-reactivity of several simple functional groups: carbon-carbon double (-C=C-) and triple bonds, nitriles, and aromatic ring structures, and defined the reactive cusp states, thereby elucidating the relative order of group reactivity under single shock conditions. The observations under shock compression will be discussed in the context of reactivity from frozen phases under static high pressure/temperature conditions.

Ping Yang: “Computational studies of bonding, spectra, and coordination of actinide species in natural environment”

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The complicated electronic structure of actinide complexes leads to their versatility of chemical reactivity, spectral and magnetic properties, and dynamical behaviors. Computational chemistry modeling can be used as an effective tool to provide a first-principle description yielding insight into these spectroscopic and dynamical properties of actinide complexes. We will discuss metal-ligand bonding and the excitation of ligand based core electrons using time-dependent density functional theory. We will also present simulation results of the dynamical behavior of actinide species interacting with minerals and water with a focus on the adsorption and complexation of uranyl at the water-mineral interface. These fundamental findings provide a solid foundation towards a more accurate understanding of the physico-chemical properties of actinide complexes in the natural environment.

Wednesday Afternoon Session Chair: Ellen Stechel, Sandia National Laboratory

Carol J. Burns: “Chemistry contributing to radionuclide monitoring and measurement”

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An expanding range of problems exist that rely on our ability to detect, quantify, and characterize radionuclides in a wide range of matrices. These applications continue to benefit from advances in measurement science (both methods and results). Long term technical challenges in radioanalytical measurements will be presented, and examples will be presented of ongoing LANL work designed to address these challenges. Specific examples will include fundamental nuclear science measurements, development of platforms for rapid assay, new tools to evaluate the chemical form of materials, and efforts to improve our understanding of environmental data.

Andrea Ambrosini: “Synthesis and characterization of oxide materials for thermochemical CO_2 splitting using concentrated solar energy”

Andrea Ambrosini, aambros@sandia.gov, Eric N. Coker, Mark A. Rodriguez, James E. Miller, Ellen B. Stechel. Sandia National Laboratories, Albuquerque, NM 87185, United States

The Sunshine to Petrol project at Sandia aims to utilize concentrated solar energy to convert carbon dioxide and water to syn gas precursors for liquid hydrocarbon fuels. Solar thermochemical CO_2-splitting is possible utilizing redox-active metal oxides:

MO_x® MO_{x-y} + y/2 O_2 (>1300˚C)

MO_{x-y} + yCO_2® MO_x + yCO (<1200˚C)

M can be, but is not limited to, Fe, Co, Ni, or Ce. Ferrite-based oxides require a support, e.g. yttria-stabilized zirconia, to be repeatedly redox-active. Ceria-based materials do not require a support but present different challenges, including high reduction temperatures and low Ce utilization. A systematic study of these oxides is underway to better elucidate microstructure, structure-property relationships, and transport behavior under high-temperature reducing and oxidizing environments. The design of in-situ experiments to investigate the chemistry under operating conditions has been a main focus. The results of these experiments and how they relate to material performance will be presented.

Eli Sutter: "In situ electron microscopy of phase behavior, melting, and crystallization on the nanoscale"

Eli Sutter, esutter@bnl.gov, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, New York 11973, United States

The promise of nanoscience lies in the fact that nanomaterials show distinct properties that are not simply scaled-down bulk characteristics. Transmission electron microscopy (TEM), providing the spatial resolution to observe individual nanostructures and follow their behavior over a wide range of conditions, is uniquely suited to study the physics governing nanomaterials.
Here, we discuss examples of the application of in-situ TEM to understanding the distinct properties of nanomaterials. Our results include identification of size effects on the phase diagram of binary alloys - key to understanding synthesis and doping of nanowires [1, 2]. We demonstrate the use of graphene shells as nano-mechanical actuators for fluid manipulation and delivery of nanoscale drops that follow crystallization pathways different from the bulk [3].

Harshini Mukundan: "Developing novel biosensing approaches for emerging infectious agents"

Harshini Mukundan, harshini@lanl.gov, Chemistry, Los Alamos National Laboratory, Los alamos, New mexico 87545, United States

With the increase in drug resistance, many pathogens are re-emerging in epidemic or pandemic potential. Development of rapid diagnostic efforts for these diseases, especially those that can detect drug resistance, is of paramount significance to global health. The sensor team at the Los Alamos National Laboratory is working on development of a waveguide-based optical biosensor platform for the detection of diseases. Such a development entails the development of not only the core sensor technology, but also accilary technology such as functional surfaces, fluorescence reporter and interfaces, that are required for effective application of any platform. Development of such an effort for the detection of biomarkers associated with several diseases, especially tuberculosis, will be discussed

Deirdre L. Olynick: "New frontiers in single digit nanofabrication"

Deirdre L. Olynick, dlolynick@lbl.gov, Molecular Foundry, Lawrence Berkeley National Lab, Berkeley, CA 94720, United States

At the Molecular Foundry at LBNL, single-digit nano refers to our efforts towards resolution, precise placement, and control of material at the sub-10 nm (single digit) scale using a combination of top-down and bottom up lithographic and assembly techniques. Electron beam exposure of resists is the mainstream lithographic technique for moderate-throughput production of accurately aligned, arbitrary shapes at high resolution. In this talk, I will discuss resolution mechanisms and limits in the highest resolution resists and how these limits affect downstream processing. New processes and materials to overcome these limits will be presented with a focus on two emerging opportunities, a dry development process which allows production of small, high aspect ratio resist features, and organometallic resists for direct patterning of high resolution metallic features. Potential applications in areas such as nanoelectronics, nanomagnetics, and plasmonics will be discussed.

Elizabeth A Glascoe: "Influence of pressure on the thermal decomposition kinetics and burn rates of the explosive HMX"

Elizabeth A Glascoe, glascoe2@llnl.gov, Joseph M Zaug, Alan K Burnham, Jon L Maienschein. Energetic Materials Center, Lawrence Livermore National Laboratory, Livermore, CA 94550, United States

In order to understand and quantify the chemistry and physics that underlie the steps involved in the thermal explosion (e.g. decomposition and burning) of an energetic material, controlled experiments have been performed. The influence of pressure on the decomposition kinetics of HMX (octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine) was studied between ambient pressure and 3.6 GPa by heating HMX in a diamond-anvil cell and monitoring the population using Fourier transform infrared (FTIR) spectroscopy. Our results indicate that at $P < 0.1$ GPa decomposition accelerates, while at > 0.1 GPa decomposition decelerates; mechanisms will be discussed. In a complementary study, the burn rates of HMX have been measured over a wide range of pressures (ambient to 0.3 GPa) and temperatures (ambient to 180 °C); the most influential variables are the pressure and sample density. Taken together the decomposition kinetics and burn rate studies provide valuable insight into the interpretation and prediction of thermal explosions.