

# Fall 06 Seminar Series Abstracts

August 30 – First day of classes

September 6

**Michael Sevilla**

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*Photo-excitation of the DNA Radical Cations: Formation of Sugar Radicals and Mechanism of Action*

Cation radicals in DNA are formed via various processes and most directly by high energy irradiation. On formation these "holes" migrate to the base guanine. In this work we show that photo-excitation of the guanine cation radical results in specific sugar radicals. These species are known to lead to DNA strand breaks. These radicals are identified by specific isotopic labelling in model systems. Theoretical work using time dependent density functional theory confirm that on excitation of the guanine cation radical the hole transfer from the guanine base to the sugar. While on the sugar we propose that a simple deprotonation occurs leading to the sugar radicals observed.

September 13

**Andrew Mason**

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*Electrochemical Microsystems Utilizing Nanostructured Biomimetic Interfaces*

The extremely high sensitivity and specificity of proteins provide an excellent source for recognition of biochemical and biomolecular agents. Recent breakthroughs in our Center for Nanostructured Biomimetic Interfaces and elsewhere have yielded a portfolio of bio-interfaces suitable for both soluble and membrane proteins, making it feasible to fabricate high-density arrays in which many different protein-based detectors are deposited on an electrode array. Utilizing electrochemical methods and integrated microsystem technologies, these arrays can be implemented on microelectronics chips for fast and continuous determination of analyte concentrations with very small sample volumes. Recent developments on an integrated bioelectrochemical microsystem platform will be presented. The system utilizes nanostructured biomimetic interfaces for continuous measurement in an aqueous sample and can be applied to applications ranging from detection of biotoxins to interrogation of the functional properties of newly expressed proteins. Example bio-interfaces and post-CMOS fabrication issues will be presented, and microsystem readout circuits, including electrochemical impedance spectroscopy, will be discussed.

Host: Xiangqun Zeng

## **September 20**

### **Colin Poole**

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*Insights into the separation mechanism for gas chromatography and beyond*

This presentation reviews applications of the solvation parameter model to gas chromatography and its use for characterizing stationary phase separation properties in terms of intermolecular interactions and how this information can be used for column selection, design and modeling biopartitioning processes.

Host: John Seeley

## **September 27**

### **Kevin Kubarych**

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*An Ultrafast Dynamical Probe of Molecular Structure: Multidimensional Infrared Spectroscopy*

Chemists have long appreciated the power of infrared spectroscopy to aid in determining molecular structure. In recent years, many groups have been working to adapt the technological breakthroughs of ultrafast laser spectroscopy to the infrared spectral region. By applying a sequence of femtosecond infrared pulses it is now possible to expand IR spectroscopy into new dimensions. I will describe our recent work in multidimensional IR spectroscopy and how it can be used to track nuclear dynamics in real time.

Host: Mark Severson

**October 4**

**David Ash**

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*Arginase: New Roles for an "Old" Enzyme*

Arginase catalyzes the hydrolysis of L-arginine to produce L-ornithine and urea. Although generally considered in terms of its role in the urea cycle, recent studies have implicated the enzyme in a number of conditions, such as asthma and erectile dysfunction syndrome. We have employed a variety of experimental approaches, including electron paramagnetic resonance, site directed mutagenesis, and x-ray diffraction, to establish structure-function relations for the enzyme. Additionally, these studies have resulted in the development of potent arginase inhibitors that have established new roles for this enzyme.

Host: Art Bull

**October 11**

**Kandace Williams**

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*The Case of a Mutator Phenotype Lurking Within the Cell Cycle*

The DNA mismatch repair (MMR) pathway contributes to the fidelity of DNA replication and recombination by correcting mispaired nucleotides and short insertion/deletion loops (IDLs). We have been investigating MMR protein expression, subcellular location, and activity in mammalian cell lines during discrete phases of the cell cycle. Results demonstrate that MMR protein expression within the nucleus, mismatch binding and nick-directed MMR activity are highest during DNA replication phase (S) and lowest throughout resting phase (G<sub>1</sub>). Despite that nuclear MMR protein concentrations are equally high during and after DNA replication (S and G<sub>2</sub>), both mismatch binding and repair activities after DNA replication are significantly lower, indicating a post-translational effect on MMR activity. We further demonstrate that specific co-localization of MutS $\alpha$  to late S phase DNA replication foci is disrupted by low level *N*-methyl-*N'*-nitro-*N*-nitrosoguanidine (MNNG) treatment that does not decrease DNA replication foci nor induce cell cycle arrest. These results suggest that alkylation damage-induced disruption of MMR activity at the replication fork may be an indirect cause of increased mutation frequency within surviving cells.

Host: Amanda Bryant-Friedrich

**October 18**

**Aaron Odom**

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*Catalytic Carbon-Nitrogen Bond Formation: Importance and New Developments*

Over 80% of the pharmaceuticals on the market contain nitrogen and installation of new CN bonds is of key importance in their synthesis. In this talk, we will discuss two important transformations for the synthesis of new CN bonds. First, we will discuss hydroamination, the addition of CH bonds to unsaturated CC bonds. Second, we will discuss the conversion of more readily available alcohols to primary amines.

Host: Ferman Chavez

**October 25 – The Isaac Eliezer Seminar**

**Dennis Curran**

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*An Introduction to Fluorous Techniques for the Synthesis of Small Organic Molecules*

This lecture features a diverse selection of recently introduced fluorous techniques unified by the theme of strategic synthesis and separation. Separation techniques include liquid-liquid extraction, solid-liquid extraction and chromatography over fluorous silica gel. Featured are fluorous monophasic, biphasic and triphasic reactions along with the use of fluorous reagents, reactants, scavengers and protecting groups in traditional, solution phase parallel and mixture synthesis. The ease of separation and product recovery make fluorous methods attractive for large scale chemistry while their speed and reliability are strong assets for small scale chemistry.

Host: Roman Dembinski

**November 1**

**Guangzhao Mao**

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*Probing Nanostructures with AFM: From Nanocrystals to Responsive*

Atomic force microscopy (AFM) is capable of providing three-dimensional topography of a solid/liquid interface with sub-nanometer spatial resolution and piconewton force sensitivity. AFM is particularly useful for the understanding and control of self-assembly by providing images and force curves during real-time transformation events from individual molecules to molecular nano-clusters and thin films. The capabilities of AFM are illustrated by two examples. One describes the template synthesis of ordered nanocrystal arrays. The second example describes the temperature-dependent phase transition and association behavior of a thermally responsive polymer.

Host: Xiangqun Zeng

**November 8**

**Peter Hoffman**

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*Solid or Liquid? – the secret lives of nanoconfined liquids*

The promise and sometimes curse of nanosystems is that systems that are perfectly well-understood at the macroscale often show peculiar properties when at least one of their dimensions is confined to the nanoscale. It turns out that simple molecular liquids are no different and over the last 20+ years nanoconfined liquids have been studied by many methods and have created a fair amount of controversy. Nanoconfined liquids are of great interest in diverse areas including cell biology, nanotribology, oil recovery, and microfluidics. After a thorough introduction, I will discuss some of our recent surprising results on several nanoconfined liquids using a state-of-the-art atomic force microscope (AFM), developed and built in our research group.

Host: Xiangqun Zeng

**November 15**

**Martin J. Stone**

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*Chemokine-Receptor Specificity: The Molecular Basis of Leukocyte Trafficking in Inflammation*

A hallmark of inflammation is the accumulation of leukocytes (white blood cells) in the inflamed tissue. The migration of specific types of leukocytes in different inflammatory tissues is regulated by the interactions of small proteins called chemokines with their receptors in the leukocyte membranes. I will describe structural studies and mutational analyses of chemokines and the development of soluble proteins that mimic chemokines receptors. Together these data can be used to develop a more detailed understanding of the factors that control chemokine-receptor recognition in inflammation.

Host: John Finke

**November 22 – No Seminar – Thanksgiving**

**November 29**

**Shulamith Schlick**

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*ESR and Polymers in the Hydrogen Economy: Direct ESR and Spin Trapping for the Detection of Radicals in Polymeric Membranes Used in Fuel Cells*

The stability of ion-containing polymers used as proton exchange membrane in fuel cells (FC) has emerged as a major problem that needs to be addressed before the transition to a hydrogen or methanol economy. The formation of reactive oxygen species such as  $H_2O_2$  and  $HO\cdot$  during catalytic processes in FC operation has been demonstrated, and their presence implicated in membrane deterioration. We have used direct ESR and spin trapping to detect radical formation in Nafion perfluorinated membranes and similar ionomers that contain pendant sulfonic groups, and in model fluorinated compounds.

Host: Mike Sevilla