THE OCTAGON

Volume 88, No. 7, October 2005 Lehigh Valley Section of the American Chemical Society

In This Issue:

Meeting Announcement:

782nd LVACS Meeting: Kutztown University

Date: Thursday October 20, 2005
Location: Kutztown University
Reception: 5:30 PM Third floor Lobby, Boehm Science Center
NCW Student Affiliates Mixer: 5:30 PM Third floor lobby, Boehm Science Center
Dinner: 6:30 PM McFarland Student Union, Room 223
Meeting: At conclusion of dinner, McFarland Student Union, Room 223
Talk: ~ 8:00 PM, McFarland Student Union, Room 223
Menu: Buffet including tossed green salad, rolls, choice of sliced roast beef with caramelized onions in mushroom sauce or vegetable lasagna w/mushrooms, lemon, shallots, and cheese; roasted red and gold potatoes and glazed baby carrots. Dessert: Chocolate cake w/mousse filling
Cost: $20.00 members $10.00 students
Contact: Donna Moore at 610-683-4447 or **moore@kutztown.edu** by Friday, Oct. 14th. Please include name and affiliation.
Directions: Directions can be found on the web at **http://www.kutztown.edu/admissions/location.shtml**

Speaker:

Dr. Nicole J. Crane

Dr. Nicole Crane grew up in Reading, PA, and graduated from Reading High School. She attended Penn State and Temple Universities before receiving her B.S. in Chemistry from Kutztown University in 2000. She pursued graduate studies in analytical chemistry at the University of Michigan, obtaining her Ph.D. in 2004 under the direction of Dr. Michael Morris. Her thesis work involved using Raman imaging to investigate biological systems. After completing her Ph.D., Dr. Crane accepted a position as a visiting scientist at the FBI Academy in Quantico, VA. Her work at the FBI labs focused on infrared imaging of fingerprints. Currently she is a postdoctoral fellow at the NIH studying several biomedical problems using infrared and Raman imaging.

Talk:

Vibrational Spectroscopic Imaging: Non-invasive Biomedical and Forensic Applications

Laboratory of Chemical Physics, National Institute of Diabetes and Digestive and Kidney Disease, National Institutes of Health, Bethesda, MD 20892

Fourier transform infrared (FTIR) spectroscopy and Raman spectroscopy are extremely complimentary and are considered to be "sister" spectroscopic techniques. Both techniques provide chemical information about organic and inorganic substances, making them ideal exploratory and identification methods for applications that deal with complex samples, such as biomedical and forensic systems. When coupled with *imaging* modalities, FTIR and Raman spectroscopies are powerful tools, providing chemically specific information as well as spatial information. FTIR imaging is faster than Raman imaging approaches and provides greater signal-to-noise ratios for the data. However, Raman imaging provides superior spatial resolution to FTIR imaging with the additional advantage that it is not confined to dehydrated samples.

In a biomedical study, Raman spectroscopic imaging is employed for the detection of transient mineral species in developing mouse calvaria. The mouse calvaria are comprised of the top most bones in the skull and the sutures, the fibrous tissue that lies between the bones. Sections, or coupons, of the calvaria are monitored *in vivo* over a 72-hour period for changes in bone mineral and bone matrix composition.

Here, FTIR spectroscopic imaging is used in a forensics study to successfully detect, non-invasively, latent fingerprints on various substrates, such as duct tape, aluminum cans, and paper money. With non-invasive detection of latent fingerprints, chemical preprocessing of the prints is not necessary. This enables additional analysis of any associative evidence contained within the print.

Chair's Message:

Greetings Fellow LVACS Members!

Thank you for a terrific "Back to School" meeting on September 22nd at Lafayette College. Chip Nataro deserves kudos for selecting a delectable menu, including that tasty peanut butter pie! Dr. Schelvis provided us with a wealth of information to help us understand DNA repair by photolyase; we thank him for his knowledge and talent to deliver the material to a wide audience.

A few administrative mentions:

1. Carol Libby announced she has starter information for Silver Circles, to promote senior and retired chemists communication. This is an excellent opportunity for our most valuable senior members to meet and exchange ideas and information. In addition, we will welcome members of Silver Circles with open arms to speak at meetings, mentor younger members, and provide us with insight and expertise on any number of topics. Please see Carol to start this wonderful group!
2. As Steve Weiner mentioned, the LVACS Senior Essay Award deadline is October 28. Please encourage your students to participate. The award is $500, plus the essay could also go towards a graduate / medical / law school application or job interview / presentation / application.
3. Our next meeting is in the midst of National Chemistry Week, and I hope everyone has plans for their respective schools. If you would like help, please let me know.

My blurbs to you would not be complete without mentioning the need for officers! Please consider running for an office. No experience necessary ☺ (can't you tell??) The section has wonderful, insightful, intelligent members, and I've seen many new faces during the last few meetings. Take the next step and accept an office position. I've learned quite a bit, met many people I now call friends, and have thoroughly enjoyed my time as a member of the Executive Committee. It's worth the little bit of extra time that an office takes, trust me.

With all sincerity, I will repeat……As always, we are here and will listen to your thoughts, ideas, and action plans for our section. We have a truly great group of people, and we can learn and grow from one another. Think about what you want from this section, and how it can happen. Let's plan and do it, okay?

I look forward to seeing you, meeting you, and interacting with you.

Cheers,

Tara S. Baney, Chair
Email: **tara_baney@merck.com**
Phone: 215-652-7486

Look For LVACS on the web at www.esu.edu/lvacs

2005-2006 Tentative Meeting Schedule

November - Lehigh University
January - Cedar Crest College (Students' Night)
February - Muhlenberg University
March - Albright
April - Moravian (Student Poster session)
May - DeSales (H.S. Teacher's night)

LVACS WANTS YOU!
CALL FOR NOMINATIONS

Do you have ideas about how chemistry should be presented or viewed in the Valley? Well then get involved and help shape our profession! Candidates are needed for 2006 elections! Anyone interested in running or nominating someone for an office please contact one of the section officers (contact information on page 7. People think being an officer is a lot of work. Well to be honest it does take some time. But not as much as you might think and it is time well spent. It's a great chance to network and meet some terrific people. It is a fabulous opportunity, especially for young chemists or chemical engineers. And for retired professionals it is a great way to stay active in and keep in touch with your profession. Help us to make the LVACS a vibrant active ACS section. Opportunity is knocking - please answer!

Congratulations to Matt Coughlin

Junior Chemistry Major at Lafayette College

Winner of the 2005
LVACS Organic Chemistry Scholarship

Matt was awarded a scholarship for his winning application and essay

Way to go!

LVACS Meeting Minutes

February 2005

The 777th meeting of the LVACS was held at Cedar Crest College on Tuesday, February 8, 2005. The meeting was attended by 51 members and their guests. Tara Baney announced that applications for the Foundation in Chemistry and the Organic Chemistry Award are being solicited. She also reminded the attendees that the annual student poster session would be held April 27th at Moravian College.

Roger Egolf gave the Treasurer's Report and indicated that the section's financial report had been submitted to the National ACS. Our money market fund, although it has nearly $27,000.00, was not producing much income due to the low interest rates.

Tara then introduced the speaker, Sharon Gerdes, the technical support consultant for Dairy Management, Inc., a trade group for the dairy industry. The title of her talk was "Do it with Dairy: Mooving and Shaking with Dairy Ingredients". Ms. Gerdes began the presentation with Functional Properties of dairy and associated products, including flavor, colour, emulsification properties (containing both hydrophobic and hydrophilic groups), water binding capacity, foaming and stabilization properties, as well as dissolution and dispersibility properties. She continued with the nutritive value and high calcium content of dairy products, transitioning nicely to Applications and Examples of milk and related dairy products.

Ms. Gerdes explained the composition of milk, which is 3.5% fat, 3.2% protein (made up of 80% Casein and 20% Whey), 4.6% carbohydrates, and ~88% moisture. She then detailed ingredients from milk and major application areas. The attendees learned in-depth about whey; various modifications, protein concentrates, and protein isolates. Also, Ms. Gerdes taught the attendees facts about lactose and it's applications in the dairy industry.

Next, Ms. Gerdes discussed new functional and nutraceutical dairy ingredients, ranging from α-lactalbumin and β-lactoglobulin to probiotics. She concluded her talk by presenting education and resources for food technologists, plus current consumer issues.

Ms. Gerdes answered numerous questions, and Tara Baney presented her with a gift from the section as a thanks for a well-delivered and informative talk. The meeting was adjourned at approximately 9:10 PM.

Respectfully Submitted,
Paul A. Bouis
Secretary, LVACS
26-September-2005

May 2005

The 779th meeting of the Lehigh Valley Section of the American Chemical Society was held on May 15, 2005 at DeSales University. The meeting was called to order by President Tara Baney at 8 PM.

Dr. Roger Egolf presented a Treasurer's Report indicating that there is $3356.96 in our checking account.

Tara Baney made several announcements. Former President Andrew Gilicinski will donate his collection of approximately 40 years of back issues of the "Octagon". Two positions are available at Merck in bulk manufacturing process engineering and facilities engineering. There will be a teachers' conference at Bucks County Community College on October 14 and 15, 2005 on the history of chemistry. A covered-dish picnic will be held at Louise B. Moore County Park on August 13, 2005.

Dr. Roger Berg announced that DeSales University holds a program of chemistry demonstration seven times each semester. The next program will be held in the Fall in late October or early November. This meeting is designated as "High School Teacher's Night". Dr. Berg asked all of the high school present to stand and be recognized.

Dr. Berg introduced the speaker for the evening, Dr. J. David Lawson, Senior Computational Chemist, Vitae Pharmaceuticals. Dr. Lawson talk was entitled "Better Living Through (Computational) Chemistry

Computational chemistry is an emerging field at the center of many overlapping disciplines, such as biology, chemistry, physics, and computer science. Computational chemistry uses computers to understand biologically important processes at the atomic level. Four major points were discussed:

Protein Structure Determination

Structural Biology and Molecular Modeling

Computational Drug Design

Computational Chemistry in the Classroom

Protein Structure Determination - X-ray diffraction patterns of protein crystals were used to elucidate the structure.

Structural Biology and Molecular Modeling - Molecular modeling is a tool for visualization of the structure. For example, visualizing the myosin crystal structure helps to understand muscle movement. Filaments slide past each other as the ATP protein undergoes a structural change.

Computational Drug Design - There are many potential compounds which haven't been tried as pharmaceuticals. Computed-aided design helps reverse engineer a drug. Many diseases can be treated by interfering with a protein's function. The computer can be used to design a structure that fits into the active site of the protein. For a given protein and liquid, a docking algorithm is used to determine the best way to fit it into the active site. Binding predictors compute the likelihood that the structure of interest will bind to the active site. Then, when a structure is found to bind, toxicology predictors help to determine if it will be a good drug.

Vitae Pharmaceuticals set up an exploratory program. They start with a piece of a drug of interest for a given target protein, then attach individual small fragments randomly. Each trial is given a score and a toxicological evaluation. Promising compounds are send to the synthetic chemists and a biological assay is carried out. Information concerning how these compounds fared is then fed back to the programmers to improve future testing.

Computational Chemistry in the Classroom - Computational chemistry is the future of the pharmaceuticals industry. It saves time and money in drug design. In the classroom, videos are appealing to young audiences. There are many free modeling programs available.

Dr. Lawson answered several questions and the meeting was adjourned at 9:15 PM

Respectfully submitted,
Dr. Pamela D. Kistler
Councilor LVACS
September 22, 2005

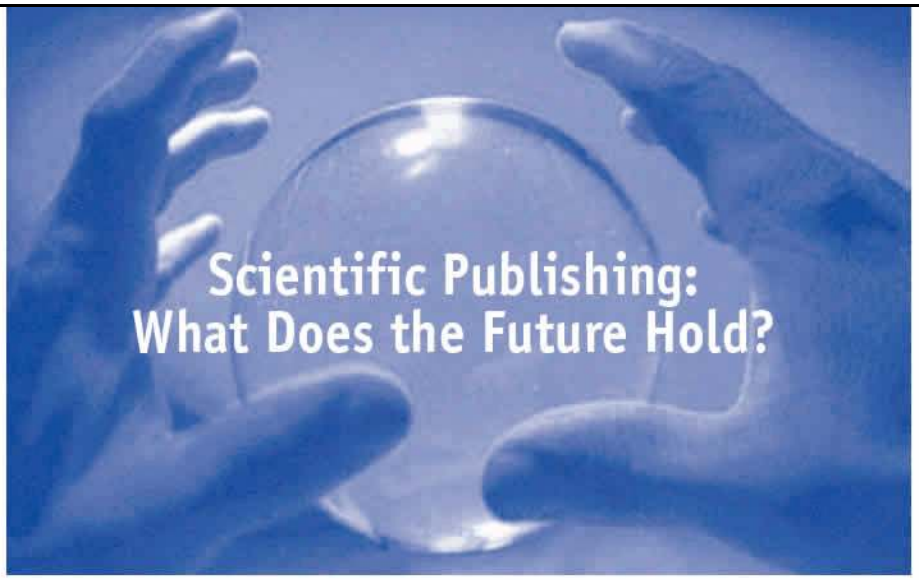
NATIONAL CHEMISTRY WEEK - THE JOY OF TOYS

Each year the American Chemical Society's (ACS) National Chemistry Week (NCW) campaign reaches millions of people with positive messages about the contributions of chemistry to their daily lives. It is the one time during the year that chemists, regardless of background, unite with the common goal of spreading the word that chemistry is good for our economy, our health, and our well-being. The date for the 2005 celebration will be October 16 – 22 with the theme, "The Joy of Toys".

It is not too late for you to join the celebration!

Some ways that you can contribute to the NCW campaign are to perform chemical demonstrations at a neighborhood school; conduct hands-on activities with children at museums, malls, or libraries; or write articles or letters to the editor of your local paper.

To find the NCW coordinator in your local section or find out more about National Chemistry Week, please visit the NCW webpage at www.chemistry.org/ncw.



Foresee Your Future at the Lehigh Conference - Saturday, November 12th

Sinclair Auditorium, Lehigh University, Bethlehem, Pennsylvania. FREE! 8:30 am - 4:00 pm. Online preregistration strongly encouraged at the conference website **http://www.lehigh.edu/scipub**

Scientific publishing is in a state of flux. Hear a set of distinguished speakers with first-hand involvement present a spectrum of views on the challenges and issues that we face as we move fully into the digital age.
Students, faculty, researchers, scientists, engineers, librarians, publishers: if you write, use, or disseminate scientific material, this conference is for you!

Julia Blixrud, Assistant Director for Public Programs,
Scholarly Publishing and Academic Resources Coalition (SPARC)
Advancing Open Access for the Public Good.

John H. Ewing, Executive Director, American Mathematical Society
Scholarly Publishing: A Century Ago, a Century From Now.

Karen Hunter, Senior Vice President, Strategy, Elsevier New York
Publishing in a Period of "Unprecedented Uncertainty"

Rosalind Reid, Editor, American Scientist Publishing,
Access and the Progress of Science

Christine M. Roysdon and Brian Simboli, Lehigh University Libraries
Whose Electronic Library Is It, Anyway?

Sponsored by the Lehigh University Chapter of Sigma Xi and Lehigh University Library and Technology Services LEHIGH

This Month in Chemical History

Harold Goldwhite, California State University, Los Angeles hgoldwh@calstatela.edu

Prepared for SCALACS, the Journal of the Southern California, Orange County, and San Gorgonio Sections of the American Chemical Society

I recently acquired through a used book outlet a copy of Volume II of the Extra Series, Numbers 5 and 6, bound with the Second Edition numbers 1 and 2, of the magazine "The New World: A Weekly Journal of Popular Literature, Science, and Music." These issues of "The New World " are dated October 1842 and March 1843 respectively and were edited by Park Benjamin, himself a writer, and published by J. Winchester.

These were enterprising gentlemen. In November 1842 the magazine published the first book of Walt Whitman, a potboiler of a temperance tale entitled "Franklin Evans or the Inebriate. A Tale of the Times". A couple of years later Winchester pirated Charles Dickens' latest novel, "Martin Chuzzlewit"and after publishing it serially in "The New World" issued the first American Edition in book form well before Harpers were able to produce the authorized edition. By now my readers are surely asking what all this has to do with chemical history? Patience, and all will be revealed. These Extra Series numbers of the magazine contain the complete texts, translated into English, of two of Justus Liebig's most important books, namely " Chemistry in its Applications to Agriculture and Physiology"; and "Animal Chemistry; or Organic Chemistry in its Applications to Physiology and Pathology."This demonstrates, I believe, an interest of the literate public in the science of the day which is strikingly in contrast to the situation in our times. A comparable publication is unimaginable in a modern general interest magazine.

In the early 1840s Liebig was regarded as the most important European chemist. He had been at Giessen for 15 years and had established the best known research school in chemistry. His work with Woehler on the benzoyl radical was already regarded as path-breaking, and his improvements in organic analysis had placed that science on a sound footing. He began to investigate chemical aspects of agriculture and, more generally, biochemical phenomena (as we would now call them) in the 1830s. It was his close friend and colleague Woehler who had discovered in 1828 the remarkable transformation of ammonium cyanate into urea, thus forging a link between inorganic chemistry and the chemistry of living organisms. Liebig decided to follow up this link.

" Chemistry in its Applications to Agriculture and Physiology"was originally presented to the British Association for the Advancement of Science as a part of a Report by Liebig on the state of organic chemistry. It was translated into English by Lyon Playfair, a distinguished chemist and, later, a noted politician. Liebig states: "I have endeavored to develop…the laws of Organic Chemistry in particular, in their applications to Agriculture and Physiology; to the causes of fermentation, decay, and putrefaction; to the vinous and acetous fermentations; and to nitrification". Liebig pays tribute to Humphrey Davy's pioneering work on "Agricultural Chemistry" which initiated reforms in farming practices in the early nineteenth century.

Liebig draws attention to the disconnect, so apparent at the time, between the views of chemists on natural phenomena of the kinds mentioned in the previous paragraph, and those of botanists and physiologists. He states:"Physiologists reject the aid of chemistry in their inquiry into the secrets of vitality, although it alone could guide them in the true path." He offers much useful advice to agriculturists, reinforcing with chemical reasoning such practices as alternation of crops, the use of natural and artificial manures. He also points out the value of chemical analysis of soils.

Liebig's views on fermentation brought him into conflict with Pasteur some years later. Liebig compared yeast with an inorganic catalyst, and said that in the fermentation of sugar solutions by yeast both the sugar and the yeast underwent decomposition. Pasteur opined that yeast was a living organism which grew during fermentation drawing its nourishment from the sugar, a view which corresponds to our present ideas.

There is much more of interest in the 63 closely printed large format quarto pages that make up Liebig's "Agricultural Chemistry" but space and time do not allow me to give more than this short abstract of its contents. In Part II, I will discuss the second of the Liebig books , that on "Animal Chemistry".

Part II

Part I of "This Month in Chemical History" described issues of "The New World" magazine from the early 1840s that contained texts of two of Liebig's most important works. It also mentioned that the publisher of this magazine pirated well known novels, including Dickens' "Martin Chuzzlewit" and it seems very likely that Liebig never received a penny from these American versions of his works. Indeed, in "An Appeal to the Reading Public" the Editor (or perhaps the Publisher) harangues against "the outrageousness and absurdity of all arrangements in favor of an International Copyright Law" alleging that it "has been urged by a certain set of aristocrats, to kill the cheap publications and to bring back the cost of books to the old standards." So much for intellectual property.

To return to chemistry the March 1843 issue of the magazine's extra series includes William Gregory's translation of Liebig's "Animal Chemistry or Organic Chemistry in its application to Physiology and Pathology". William Gregory was Professor of Medicine and Chemistry at the University of Aberdeen. Liebig begins by paying

tribute to Lavoisier as the founder of the new science of chemistry. Indeed, as Frederick Holmes and Jean-Pierre Poirier have pointed out in recent books about Lavoisier, the French chemist can also be viewed as the first scientific biochemist.

Liebig draws parallels between the physiology of humans and of other animals and suggests that the initial objects of physiological studies should be the understanding of what we might call the mechanical aspects of physiology. He decries "the efforts of philosophers, constantly renewed, to penetrate the relations of the soul to animal life", concluding that such efforts have retarded the progress of physiology.

A penetrating analysis of animal heat refines the conclusions of Lavoisier on respiration as its source. "Even when we consume equal weights of food in cold and warm countries, Infinite Wisdom has so arranged that the articles of food in different climates are most unequal in the proportions of carbon that they contain. The fruits on which the natives of the south prefer to feed do not in the fresh state contain more than 12 percent of carbon, while the bacon and train oil [!] used by the inhabitants of the arctic regions contain from 66 to 80 percent of carbon."

A section on the metamorphosis of tissues has some interesting observations: "…albumen, fibrine and caseine … contain exactly the same proportions of organic elements. When …[they] are dissolved in a moderately strong solution of caustic potash, and the solution is exposed for some time to a high temperature, these substances are decomposed. The addition ofacetic acid to the solution causes, in all three, the separation of a gelatinous translucent precipitate, which has exactly the same characters and composition, from whichever of the three substances.. it has been obtained. Mulder [gave] to this product of the decomposition of albumen &c. by potash the name of proteine [from the Greek word meaning "I take the first rank"].

Further sections of this fascinating book include analysis of the phenomena of motion in the animal organism; a theory of disease which depends heavily on the idea of vital force; and an appendix that contains the analytical evidence underpinning Liebig's conclusions. The whole text covers 48 pages of closely printed quarto paper.

As a bonus the bound volume in which these chemical texts are found also includes George Borrow's book on "The Bible in Spain"; the first (no doubt pirated) American edition of a novel "The Jewess; A Tale from the Shores of the Baltic"; miscellanea on a vast range of subjects including the American politics of the period; and two long scientific articles, the first, by M. Arago, the distinguished French astronomer, and the second by Thomas Dick, on comets. A brilliant comet appeared in 1843, eliciting, probably from the pen of Noah Webster, the following comment in the New Haven Herald: "The present comet is considered as a very brilliant phenomenon, but it is far inferior to that which I saw when young, either in 1769 or 1770." Things were always better in the old days.

Question of the Month

(A Hollywood theme)
How did the invisible man obtain his invisibility?
Come to the October meeting for the answer

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