

# ChemNotes

{ TUFTS UNIVERSITY CHEMISTRY DEPARTMENT }

2000 • FALL



Christy DiCologero  
looking into the ultra-  
high vacuum chamber.

## DUAL MISSION

## Research and Education

The Tufts University Department of Chemistry continues its commitment to the dual mission of education and research.

### RESEARCH

#### *Arthur L. Utz*

Professor Utz joined the Tufts Chemistry Department in 1994 following graduate training at the University of Wisconsin-Madison and a postdoctoral appointment at the Massachusetts Institute of Technology. He was recently promoted to the rank of Associate Professor of Chemistry. His research group at Tufts conducts experiments that reveal the mechanistic basis for important reactions occurring on the surface of transition metal catalysts.

In many chemical reactions, reagents take part in a richly choreographed script that brings reactants together, allows some chemical bonds to break while others form, and then produces new chemical species as the reaction proceeds. A mechanistic understanding of this chemical dance provides the insight necessary to manipulate and control the outcome of the reaction. Modern organic chemistry provides a striking example of this approach.

Unfortunately, such understanding is rarely, if ever, available for reactions on solid surfaces. It is generally known that heterogeneous catalysts lower activation energies by forming new adsorbate-surface bonds while other bonds break. It is much less clear which molecular contortions accompany this transformation of reactants into products.

*Continued on page 2*

## Chair's Corner

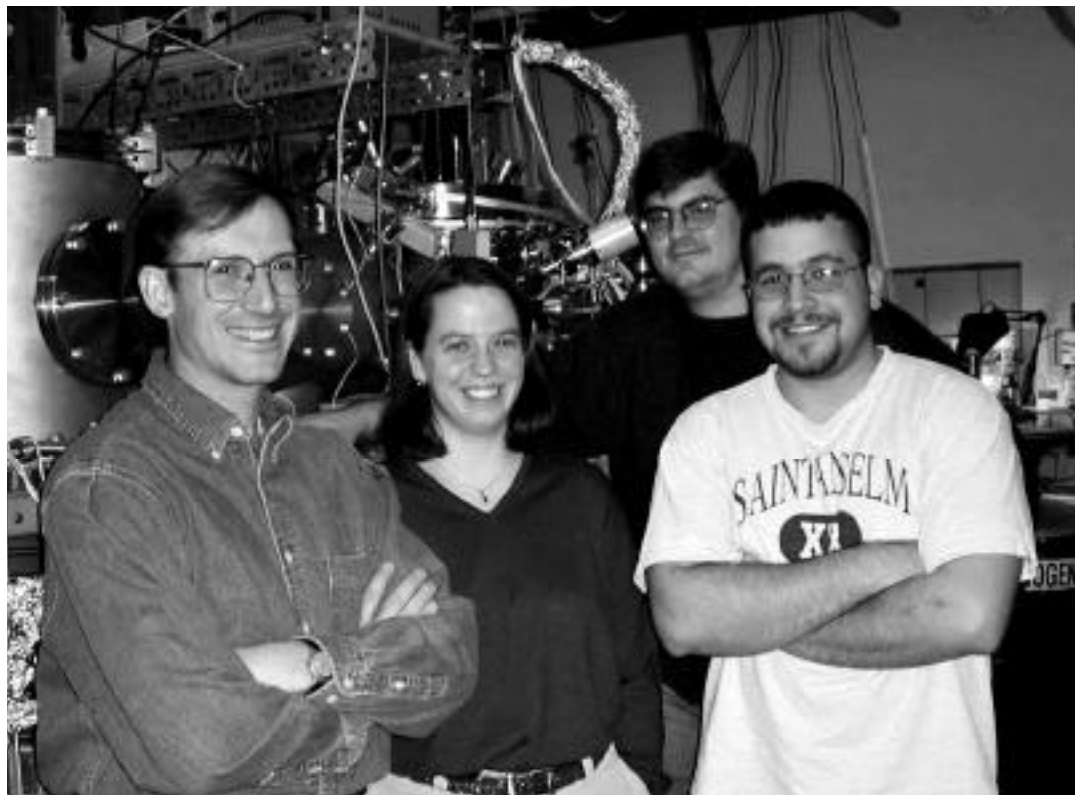
MARY SHULTZ

This fall Professor d'Alarcao stepped down as chair of the department to take a well-deserved sabbatical leave. The department has taken some significant steps forward under Professor d'Alarcao's leadership. We expanded the regular offerings in our introductory chemistry program with the implementation of the Chemistry 11/12 sequence (more about this below). This year we graduated a record number of Ph.Ds with eleven students graduating — nearly one-quarter of the total for Arts and Sciences. These eleven students came from eight different research groups. The department remains strongly committed to both sides of its dual mission of research and teaching. Importantly for the future of the department, we are extremely pleased to announce that Professor Utz has achieved tenure, becoming a permanent part of our faculty. Congratulations!

The chemistry 11/12 sequence has just completed its first two cycles and early results are very positive. Chemistry 11/12 was designed as an introductory chemistry course for those with strong preparation. This class features seminar style presentations by practitioners of the art designed to illustrate how the chemistry

*Continued on page 8*

Insights gained from this work have led to a strategy that controls chemistry on surfaces.



Utz group: Art Utz (1.) with graduate students Christy DiCologero, Richard Smith and Deno DeSesto.



Pioneering experiments conducted in the Utz group have provided chemists with a new way to probe how dynamical motions drive reactions at the gas-surface interface.<sup>1</sup> These experiments use infrared laser light to impart molecules with a precisely known molecular motion prior to their impact with the surface. Tuning the light into resonance with different absorption transitions selects the molecular motion under study. Sensitive analytical techniques then quantify the efficacy of that motion in promoting dissociation and adsorption of the gas-phase reagent onto a surface. Those motions that best promote reactivity resemble the critical molecular deformations needed to access the transition state for the reaction.

Initial experiments explore the mechanism for methane dissociation on a nickel surface. In a typical industrial reactor one methane molecule reacts for every billion molecules incident on a catalyst surface. The mechanistic origin for this low reactivity has been the subject of extensive debate. On one hand, C-H bond extension would appear necessary to produce the surface-bound CH<sub>3</sub> and H dissociation products. Alternately,

the reaction barrier may arise from the need to bend the tetrahedral methane molecule and expose the central carbon atom to the nickel orbitals that form the Ni-CH<sub>3</sub> bond. In both of these pictures, energy required to distort the methane molecule into a favorable geometry for reaction contributes to the activation barrier.

State-resolved experiments provide a direct experimental test of these ideas. Infrared laser excitation of a C-H stretching vibration prepares reactants whose C-H bonds are already stretched as they approach the surface. This excitation enhances methane dissociation on nickel by a factor of 1600 relative to molecules in their ground vibrational state.<sup>2,3</sup> Laser excitation of a bending vibration is less effective than C-H stretch excitation in promoting reactivity. The differing efficacy for these two forms of vibrational energy leads to three important conclusions regarding methane dissociation: 1) the high activation barrier arises, at least in part, from a need to stretch a C-H bond, 2) bending excitation is less important than stretching excitation and 3) energy deposited into different vibrational motions can influence reactivity in different ways.

1 P. R. McCabe, L. B. F. Juurlink and A.L. Utz, *A molecular beam apparatus for eigenstate-resolved studies of gas-surface reactivity*, Rev. Sci. Instrum., **71**, 42 (2000).

2 L. B. F. Juurlink, P. R. McCabe, R. R. Smith, C.L. DiCologero and A.L. Utz, *Eigenstate-Resolved Studies of Gas-Surface Reactivity: CH<sub>4</sub> (n<sub>3</sub>) Dissociation on Ni(100)*, Phys. Rev. Lett., **83**, 868 (1999).

3 L. B. F. Juurlink, R. R. Smith, P. R. McCabe, C. D. DiCologero and A.L. Utz, *in preparation*,

These experiments are not limited to studies of vibrational effects. Preparing reactants in selected rotational states reveals how molecular rotation and orientation influence reactivity.<sup>4</sup> Such experiments suggest that the surface may exert a torque and reorient, or “steer incident,” methane molecules from unfavorable approach geometries into orientations more favorable for reaction. Experiments are currently underway to further test this idea.

Insights gained from this work have led to a strategy that controls chemistry on surfaces.<sup>5</sup> The laser excitation process results in a highly collimated stream of reactive molecules impinging on the surface. This innovation, which is the subject of a U.S. patent application, could find important uses in semiconductor and materials processing where such a source of reagents would permit etching or growth of surface structures with extremely steep walls.

Research in the Utz group is supported by a grant from the National Science Foundation. You can learn more about this work, take a virtual laboratory tour, and find recent publications at the Utz group website, <http://www.tufts.edu/~utz/index.html>

## EDUCATION

### *Teaching with Technology*

A new initiative called “Teaching with Technology at Tufts” (TTT) sponsored by Academic Technology and the Center for Teaching Excellence brings technology into the classroom. In its first year, six fellowships were competitively awarded to diverse projects ranging from The Sungeati Epic (History) to Molecular Visualization (Chemistry and Biology). Krishna Kumar was one of the six fellows for 1999. His project titled “Scientific Visualization in Organic and Biological Chemistry” has led to the development of a web site which allows interactive learning. A representative database of three dimensional organic molecules has been compiled and these can be rotated and examined in three dimensions on any personal computer across campus. Furthermore, enzyme and chemical kinetics are explained by intuitive plots with user controlled data input. The site is now being expanded to include tutorials on enzyme and protein structure, again with molecular models that allow examination in 3-D space. This initia-



Krishna Kumar using Chime® to display molecular structures.

tive serves to exemplify how the much hyped concept of interactivity can be applied to genuine pedagogic ends.

### *Critical thinking in general chemistry*

Jonathan Kenny has been involved in the initiative to teach critical thinking in General Chemistry courses for scientists and non-scientists. The aims are to claim the students’ attention during their introduction to science and to teach them the types of thinking they will need to develop scientific minds. They learn the use of metaphor, testing of hypotheses and inductive/deductive reasoning. In Spring 2000 semester, Kenny taught “Critical Thinking and Writing” in Chem 8, an environmental chemistry course for nonscience students. Student journals, with entries based on articles from current periodicals, form a major component in this course. The journals help students accomplish several important pedagogic goals, including connecting classroom learning to real-world issues and events, establishing connections between students’ own disciplines and the natural sciences, especially chemistry and using the integrative power of regular writing assignments to help students establish their command of the course material.

A critical thinking component, which utilizes Giere’s six-step program for evaluating theoretical hypotheses was added to the course. In addition to using this program to evaluate a common article assigned to the whole class, students are invited to use it regularly in their journal entries, when the article they have selected is amenable to such an analysis.

The journals help students accomplish several important pedagogic goals, including connecting classroom learning to real-world issues.

4 L. B. F. Juurlink, R. R. Smith and A.L. Utz, *The role of rotational excitation in the activated dissociative chemisorption of vibrationally excited methane on Ni(100)*, Trans. Faraday Soc., in press, (2000).

5 L. B. F. Juurlink, R. R. Smith and A.L. Utz, *Controlling Surface Chemistry with Light: Spatially Resolved Deposition of Rovibrational-State-Selected Molecules*, J. Phys. Chem. B, **104**, 3327 (1999).



# Faculty and Staff News



**Michelle DeBakey** joined the staff in the front office last May. A graduate of Emerson College, Michelle brings to the department a very interesting background. She is an independent film maker currently working on a video documentary called *Quality of Life*. She has utilized this expertise to become a valuable resource for media-related projects.

**Dave Wilbur**, Instrumentation Specialist, also joined the department last May. His substantial NMR experience has added quality to the department's research endeavors. Since his arrival, he has developed training sessions for the NMR and SEM and supervised the successful installation of the EPR.

**David Walt** initiated the Outreach Program in 1989 to introduce students to science at an early stage in their education. Initially, Walt took a few volunteers from the organic chemistry class and visited local elementary schools. The program has since expanded and is now under the direction of **Sarah Iacobucci**, manager of the teaching laboratories. Experiments are selected to demon-

strate chemical principles with safety as a key criterion for selection. There are multiple benefits to the program including an opportunity for Tufts undergraduates to learn about teaching while providing an enriching science experience for elementary school students. Women are especially encouraged to volunteer for the project to serve as role models for young girls.

**Chris Morse**, lecturer for the Chemistry Department, is also currently serving as the Graduate Training Coordinator at Tufts. This position is the second-in-command at the Center for Teaching Excellence and is designed to create and organize all faculty development opportunities for current graduate students. The goal is to make them better educators and more attractive candidates in the academic community.

The American Chemical Society theme for 1999 was "Celebration of Color." As an invited speaker, **Mary Shultz** spoke about bringing colorful, cutting edge research into the introductory chemistry curriculum with nanoscaled materials. Gold, the color, arises from squeezing the nearly free electrons in

the metal into a small space. The regular array of the atoms in the cluster, and the essentially free electrons make this an excellent system for teaching many fundamental properties of electrons. As computer components scale to smaller and smaller size to increase speed and reliability, the structures are predicted to approach nanoscale within the decade. Hence, understanding conductors and contacts on this scale is a subject of intense investigation.

At the Gordon conference on vibrational spectroscopy which featured an evening devoted to Sum Frequency Spectroscopy, **Mary Shultz** presented her group's recent work on probing the structure of water and ammonia at the aqueous/air interface.

**Professor Shultz** also gave an invited presentation at the March ACS meeting in San Francisco which featured the research projects completed by students from the undergraduate physical chemistry laboratory – synthesis of gold quantum dots and discovering a transition state analogue for alcohol dehydrogenase. She also gave a presentation at the Telluride Conference on Water titled,



Scenes from the summer cookout to welcome new graduate students.



“Water in the confined space of the Air/Water Interface” and chaired a session on condensed water in the atmosphere.

**David Walt** is in his fifth year as the executive editor for *Applied Biochemistry and Biotechnology*.

**Clemens Richert** won the ORCHEM 2000 award from the Organic Division of the German Chemical Society. He was also a speaker at the Frontiers of Chemistry Symposium at Seon, in July.

At the ACS Meeting in San Francisco, **Elena Rybak-Akimova** gave an invited lecture at the symposium on molecular mechanics of coordination compounds.

**Krishna Kumar** is the Tufts University nominee for the PEW Science Scholar Award.

**Sam Kounaves** chaired the Gordon Research Conference on Chemical Sensors in Ventura CA. He also gave an invited lecture on Planetary Chemical Analysis: In-Situ Electroanalysis of the Soil on Mars). Kounaves and his research team,

who have been involved in the research and development of MECA, a robotic chemical laboratory for analysis of the soil on Mars have been awarded two new grants from NASA. The grants were awarded by NASA's Space Life Sciences Division Advanced Human Technology Program (AHST) in support of research and development of technologies that will allow humans to explore and live in space safely and efficiently.

*Subsurface Contaminant Monitoring Using Laser Fluorescence* was written by **Jonathan Kenny** and co-authored by **Jane Pepper**, **Andrew O. Wright**, and **Yu-Min Chen**. The book was published by Lewis Publishers in January 2000.

**Karl Illinger** spent his sabbatical leave, Spring 2000, exploring *ab initio* computational methods to analyze the infrared radiative properties of technological gases. Building upon previous work on the fluoroethanes, he extended these studies to more complex molecules of the type that are currently entering the arena of chlorofluorocarbon replacements. While these

replacements evade the problem of ozone depletion in the stratosphere caused by chlorofluorocarbons, they retain the intense absorption in the infrared, and hence remain potential greenhouse-effect gases. His research has previously shown that *ab initio* calculations of the instantaneous infrared forcing ( $W m^{-2} ppbV^{-1}$ ) are competitive with experimentally determined values. Furthermore, *ab initio* computations at a sufficiently high level of the theory, in addition to providing reliable numerical estimates, also permit an analysis of how molecular properties vary with molecular structure. His recent work has further demonstrated the cogency of a model for infrared radiative properties based on atomic polar tensor analysis. The ability to predict infrared radiative, as well as other, molecular properties by *ab initio* computations can then serve as the scientific basis for the molecular engineering of technological gases.

# Student News

## Undergraduates

### Chemistry Major Awards 1999–00

#### The R.M. Karapetoff Cobb Award

Shari Cohen  
Melissa Passino

#### The M.D. Angell & H.B. Durkee Scholarship

Rebecca Noll

#### The Durkee Scholarship

Michael Hillinski  
David Stitelman

#### The Max Tishler Prize Scholarship

Shari Cohen  
Nicholas Spinelli

#### Howard Sample Prize in Physics

David Stitelman

#### Audrey Butvay Gruss Science Award

Rebecca Noll

#### The Theresa McDermott Carzo Award

Susan Meaney

#### The Prize Scholarship of the Class of 1882

Bradley McGregor

## Graduate Students

At The Gordon Conference on Vibrational Spectroscopy, **Carolyn Gin** (Shultz) presented a poster featuring water and ammonia in small clusters in  $\text{CCl}_4$ . **Danielle Simonelli** (Shultz) gave an invited talk at the ACS meeting in Washington, D.C. on "Ammonia at the Air/Water Interface — a Probe for Water."

Last summer, the Chemistry Department teamed up with the Wright Center for Science Education and hosted a workshop for twenty-five master teachers from all over the United States. **Magdalena Tsakova**, from the American College of Sofia in Bulgaria, led the workshop giving an international perspective to the quest of exciting young minds about the study of chemistry. In the chemistry department, **Professor Shultz**, several graduate students, **Colleen Bleczinski**, **Christine Jaworek**, **Cheryl Schnitzer**, **Danielle Simonelli**, and local high school student Kimberly Shultz led participants in hands-on experiments using color, toys, and other tricks to excite secondary students about chemistry.

## Semester Achievement Awards

### Spring 1999

TEACHING ASSISTANT:  
William Connors  
STAFF: Minh Nguyen  
FACULTY: Arthur Utz

### Fall 1999

TEACHING ASSISTANT:  
Georgia Marnera and  
David Turner  
STAFF: Michelle DeBakey  
and David Wilbur  
FACULTY: Chris Morse

### Spring 2000

TEACHING ASSISTANT:  
Henning Groenzin  
STAFF: Minh Nguyen  
FACULTY: Marc d'Alarcao

## Doctoral Degrees Awarded

### 1999

**Rich Breitkopf** (Haas) "Novel MOCVD Routes to Solid State Ionic Materials"

**Todd Dickinson** (Walt) "Cross-Reactive Fiber-Optic Sensor Arrays in the Design of an Artificial Nose"

**Karri Michael** (Walt) "Development of High-Density Optical Fiber Arrays: New Designs and Applications in Microscopy, Microfabrication and Chemical Sensing"

### 2000

**Charles Amass** (Haas) "An NMR Study of Lithium Reacting with N, N'-bis[2-(dimethylamino) ethyl]-N,N,-dimethyl 1,2-Benzenedimethanamine, A Model compound of Lithium-Graphite Intercalation."

**Colleen Bleczinski** (Richert) "Synthesis, Selection, and Characterization of Oligonucleotide Hybrids with Increased Target Affinity and Selectivity"

**Christine Jaworek** (d'Alarcao) "Synthesis of Inositol Phosphate Glycons"

**Ludo Juurlink** (Utz) "Eigenstate-Resolved Measurements of Methane Dissociation on Ni(100)"

**Alexander Kornienko** (d'Alarcao) "Practical Enantiospecific Synthesis of Differentially Protected Cyclitols"

**Melissa Nolan** (Kounaves) "Microfabricated Iridium Arrays: Failure Mechanisms, Investigation of the Hg-Ir Interface and their Use in Cu or Hg Determination"

**Jane Pepper** (Kenny) "Design and Application of a Multichannel Laser-Induced Fluorescence System for Environmental Monitoring"

**David Sarracino** (Richert) "Inter- and Intramolecular Complexes of Single Stranded Oligonucleotides with Peptides and Peptide Analogs"

**Cheryl Schnitzer** (Shultz) "Sum Frequency Generation of Water on Inorganic Acid and Salt Solutions"

**Sigurdur Smarason** (Robbat) "Advances in Cone Penetrometry and Fast Gas Chromatography/Mass Spectrometry for the Sampling and Analysis of Subsurface Pollutants"

**Angela Zapata** (Robbat) "Development and Performance Enhancement of a Microwave Induced Plasma Mass Spectrometer for Gas Chromatographic Detection"

## Master's Degrees Awarded

### 1998–99

**Christa Bock** (Walt)  
**Roberto Bosco** (Kenny)  
**Gregory Hall** (Utz)  
**Georgia Marnera** (d'Alarcao)  
**Laura Taylor** (Walt)  
**David Turner** (d'Alarcao)

### 1999–2000

**Kendra Dombi** (Richert)  
**William Connors** (Richert)  
**Dahai Ren** (Walt)  
**Christiane Struve** (Shultz)  
**Xiarong Tang** (Walt)  
**Charles Tetzlaff** (Richert)



# { INSTRUMENTATION }

**T**HE NATIONAL SCIENCE FOUNDATION GRANTED AN award for “Purchase of an EPR Spectrometer for Inorganic Chemistry Research”, in 1999. This award from the Chemistry Research Instrumentation and Facilities (CRIF) Program of NSF was supplemented by matching funds from Tufts University and allowed the Chemistry Department to purchase a modern electron paramagnetic resonance (EPR) spectrometer from Bruker.

An electron paramagnetic resonance (EPR) spectrometer is used to obtain information about the molecular and electronic structure of molecules. The EPR method provides unique information about the electronic structure of molecules having unpaired electrons.

Most transition metal compounds fall into this category. The method may also be used to obtain information about the lifetimes of free radicals which are often essential for the initiation of tumor growth and/or a variety of chemical reactions.

An EPR method provides an invaluable tool in characterizing paramagnetic compounds, in particular, free radicals and open-shell transition metal complexes. In coordination chemistry, the method is very helpful in determining the oxidation and spin state of the central metal ion, the geometry of its coordination sphere, the details of the electronic structure of the complex, and the extent of spin-spin interactions and/or spin delocalization in multinuclear compounds. The availability of an EPR technique is often critical for inorganic chemistry research, since the traditional NMR method fails for most of the paramagnetic samples because of enormous line broadening. The absence of an EPR instrument at Tufts University severely limited the progress in inorganic chemistry research, as well as in related areas of biomedical and materials science (the areas of focus at the Chemistry Department).

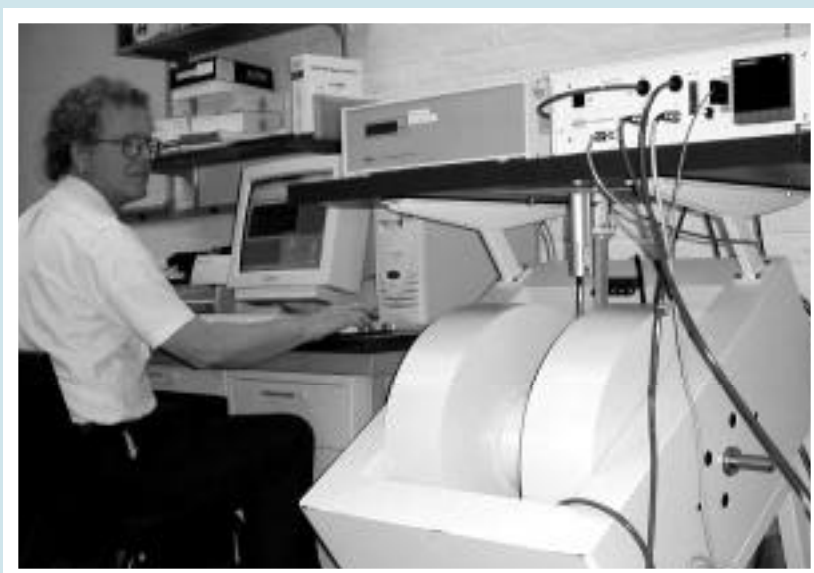
Junior faculty Elena V. Rybak-Akimova will be the primary user of this instrument, which will facilitate her studies on transition metal coordination chemistry and the design of selective redox reagents and catalysts. In addition, she will investigate magnetically coupled materials, five-coordinate species with a vacant site at the metal ion, and molecular tweezers.

The Chemistry Department has been highly successful in building on its strengths in the focus areas of environmental, materials, and biomedical chemistry. The Tufts administration and the department faculty continue to work together to produce an excel-

lent research environment by attracting young scientists to the faculty and providing much needed infrastructure support, primarily in the form of fully renovated laboratories and physical facilities.

While significant recent acquisitions have been made in the area of research instrumentation (e.g. new console for the NMR AM 300 spectrometer, electron microscope, MALDI TOF mass spectrometer, AA), in the area of characterization of paramagnetic compounds we have fallen behind. The new EPR spectrometer will significantly improve the infrastructure for chemistry research and strengthen the existing collaboration between the departments on the Medford campus. In fact, the need for an EPR spectrometer is even clearer, when the instrumentation currently available is consid-

ered in the context of related instrumentation available for chemistry research at other departments on campus. While there are numerous tools for characterization of organic molecules and organic/inorganic bulk materials in the department, the capabilities of characterizing individual paramagnetic molecules are limited. At the same time, extensive instrumentation for magnetic susceptibility measurements, including SQUID magnetometer, is available in the Physics Department and can be



Dave Wilbur, Instrumentation Specialist, at the EPR spectrometer.

used for chemical research on magnetically coupled materials on a time-shared or collaborative basis. EPR data will complement the results of magnetic measurements and help in interpretation of ground and excited spin states in such materials. Electron paramagnetic resonance is also indispensable in collaborative research with the Biotechnology Center in the field of biomimetic materials, in particular, in catalytic peroxidase-mimicking oxidative polymerization of phenols. The mechanistic studies of the transition-metal catalyzed redox reactions are vitally important for several research projects currently underway in Rybak-Akimova's group. EPR spectrometer will provide the missing link between the kinetic data and their mechanistic interpretation, giving the much needed information on the electronic structure of catalytically active intermediates. The availability of an EPR instrument will also provide new insights into the current projects in several other research groups.

The instrument will be actively used in teaching and training of undergraduate and graduate students and postdoctoral researchers. All members of Rybak-Akimova's group will be involved in extensive EPR work in the course of their training. Students who will be

*Continued on page 9*

# Class notes

**1979** Maria Campos Toft, a graduate of Penn State College of Medicine, is an Assistant Professor of Pediatrics at UMDNJ University Hospital in Newark, N.J. She has five children (ages 3, 5, 8, 10, and 12), is a faculty member at UMDNJ and is very involved with her children's activities.

**1994** Eric Farbman (BS 1994-MS 1995), a graduate of New Jersey Medical School is starting his neurology residency at the University of Pittsburgh Medical Center.

**1994** Jennifer Sloan is currently employed at Ascent Pediatrics, a drug development company dedicated to addressing the unmet medical needs of children through the development of differentiated, proprietary products. Jennifer was married at Goddard Chapel in 1997 to Jeremy Slotnick, also a Tufts graduate.

## Where are they now?

**Melissa Nolan (Ph.D. 1999)**  
Post-Doc, Northwestern University

**Bizuneh Workie (Ph.D. 1996)** Asst. Professor, Jackson State University

**Wen Deng (Ph.D. 1995)** – R&D Chemist, Copley Pharmaceutical, Inc.

**Timothy Zhaohui Liu (Ph.D. 1994)**  
Research Chemist, Perkin-Elmer-Biosystems

**Stefanos K. Intzes** UG Research 1999/2000 – University of Oxford Medical School.

**Emily M. White** UG Research 1996/97 – Ohio State University Chemistry Ph.D. Program

**Steve Baldelli (Shultz)** Post Doc w/ Somerjai, Berkeley

**Colleen Bleczynski (Richert)**  
Post Doc Columbia

**Chris Jaworek (d'Alarcao)** Faculty Position at Emmanuel College

**Ludo Juurlink (Utz)** Post doc in Holland

## IN MEMORIAM

.....

CIRCA 1935

**Thomas Glynn, Jr.**

DIED AT THE AGE OF 86

IN RIDGEWOOD, N.J.

HE WAS

A CHEMIST AT LEVER

BROTHERS FOR

FORTY YEARS.

## Chair's Corner

*Continued from page 1*

that students are learning is used in cutting-edge developments in the field. The first group of students through the sequence has just concluded the process of choosing majors and nearly one-quarter choose a major in our department – chemistry, biochemistry, or chemical physics. More than 85 percent of the alums of this class choose a major in one of the science or engineering disciplines. Although the direct goal of the course is to teach students chemistry, it appears that the combination of a higher level discussion made possible by the student's strong preparation and the prominence of the relevance of



Mary Shultz

chemistry to current real world problems has also enticed a large portion of the class to delve further into the subject.

Our major challenges in the coming year are to add to the faculty and continue the process of raising funds for completion of the renovation

of Pearson. For the faculty position, we seek candidates with research interests that augment our focus areas: biomedical, environmental, and materials. Alumni are often excellent sources of contacts for prospective faculty. I urge you to bring our search to the attention of individuals dedicated to dual careers in teaching and research.

If you are in the Boston area, I invite you to stop by to see first hand what support from friends of the department has done for the department. Several research labs have been renovated providing excellent facilities for the groups housed therein. The new classroom is the envy of the campus with a full array of AV equipment and comfort-

able surroundings. Acquisition of a major influx of modern equipment for the physical chemistry laboratory is nearly completed. This equipment is supported by a grant from the National Science Foundation, a grant greatly assisted by the modern facility. All but our most recent alums will have difficulty recognizing this facility and we thank all of you who contributed to make this possible. We also thank you in advance for your assistance in seeing us through the remainder of this renovation project.

Mary Shultz  
Chair



## Instrumentation

*Continued from page 7*

joining the group in the future will also acquire experience with the EPR technique. Although the instrument will primarily be used as a research tool, it will occasionally be used in teaching the Chem165 (Physical methods in Inorganic Chemistry) course – a graduate level course (open for advanced level undergraduates) developed by the Co-PI. As a result, a number of students will become aware of the real potential of the EPR method, and will appropriately use the technique in their research at Tufts, and in their future professional careers.

The students will enter the work force with a hands-on appreciation for the capabilities of the EPR technique, one of the most powerful methods of characterization of paramagnetic compounds and materials.

The Bruker EMX spectrometer, is a relatively simple, although very powerful research tool. The instrument is equipped with a temperature controller needed for low-temperature and variable-temperature experiments. In addition to excellent technical charac-

teristics of the EMX spectrometers (in particular, homogeneity and stability of magnetic field, high resolution and sensitivity), the system has several other attractive features, including modular design which allows for a modification and upgrade of individual blocks and provides the flexibility over a long period of operation, and an IBM-compatible PC interface which greatly simplifies instrument operation and data processing. The use of MS Windows environment for the EMX spectrometer software makes the operation of the instrument intuitive and user-friendly, and provides an open interface to peripherals and other software packages. This is possible due to parallel processors (transputers) in each of the module, which perform real-time multi-function operations such as field sweeps without active PC participation. This architecture is particularly important for new or inexperienced users of the EPR spectrometer. The usually long learning curve for the students studying the EPR method is expected to become significantly shorter due to MS Windows interface used by every student on an everyday basis. As a result, more graduate and undergraduate students will operate the spectrometer and acquire experience and expertise in EPR technique.

### Donors to the CHEMISTRY FUND for support of renovations

Ms. Carolyn Allen  
Dr. Anthony Bevilacqua  
Mr. Merrill Bleye  
Dr. Jon Michael Brooks  
Dr. Richard Brown  
Mr. Warren B. Brown  
Ms. Janet Cares  
Dr. Tae Cho  
Dr. Richard Cottiero  
Dr. Harold Freedman  
Mr. Mitchell Goldman  
Mr. Clifford Harrington  
Dr. and Mrs. William Koster  
Mr. Jack Krol  
Dr. J.B. Liska  
Dr. Bruce Marshall  
Mr. John McGonagle  
Dr. Robert O'Brien, Jr.  
Ms. Mary Passalacqua  
Mr. Joseph Peppe  
Mr. Richard Popovic  
Ms. Lisa Reindorf  
Mr. Martin Robbins  
Mrs. Elizabeth Tishler  
Mr. John Young

## The Tufts Chemistry WEB site! <http://chem.tufts.edu>

**O**UR SITE PROVIDES INFORMATION SUCH AS COURSE LISTINGS, current course material, degree requirements, faculty/staff/student info, the graduate program, special events, links to other chemistry resources, an on-line historical archive, back issues of ChemNotes, and more detailed information about the exciting and ongoing research being carried out by our faculty. The hope is that this resource will provide information for prospective graduate students and alumni and will eventually contain links to many valuable chemistry resources within the department and throughout the world. Check us out and see what is currently going on in the department. You can access our site at: <http://chem.tufts.edu>

We are still collecting information for several new areas including "Alumni Page" where we would like to list as many of you as possible. We would like to include not only names and e-mail addresses but items of interest and WWW links to Alumni pages and your areas of current employment or involvement. So please write or e-mail us if you would like to be included. Let us know where you are and what you are doing!

*The web site was created and is maintained by Professor Samuel Kounaves ([skounave@at.tufts.edu](mailto:skounave@at.tufts.edu)).*



# Seminar Series

SEPTEMBER 12

**Prof. Gregory Petsko**

Brandeis University  
*The Trouble with Hydrogens*

SEPTEMBER 19

**Prof. John Warner,**

UMass, Boston  
*Pollution Prevention using Molecular Recognition and Self Assembly: An Example of Green Chemistry*

SEPTEMBER 26

**Prof. John Tully**

Yale University  
*Chemical Dynamics at Surfaces*

OCTOBER 3

**Prof. Jeffrey Roberts**

University of Minnesota  
*Chemistry at a High-Traffic Interface: Uptake of Small Organic Molecules by Liquid Sulfuric Acid*

OCTOBER 17

**Prof. James Rusling**

University of Connecticut  
*Active Biomolecular Films on Electrodes*

OCTOBER 24

**Prof. Sean Decatur**

Mount Holyoke College  
*Probing Peptide Conformation and Dynamics via Isotope-Edited Infrared Spectroscopy*

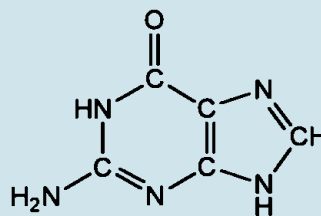
OCTOBER 31

**Prof. Sanford Asher**

University of Pittsburgh  
*Crystalline Colloidal Array Materials: Chemical Sensors and Electrooptical Applications*

NOVEMBER 14

**Prof. Robert Corn,** University of Wisconsin Madison  
*DNA Computing at Surfaces*



NOVEMBER 21

**Dr. David Casebier**

Arqule  
*Combinatorial Chemistry Applied to Lead Optimization: Numbers are Not Enough*

NOVEMBER 28

**Prof. Ricardo Metz**

UMass, Amherst  
*Photofragment Spectroscopy of Reaction Intermediates and Multiply Charged Ions*

DECEMBER 5

**Prof. Judith Herzfeld**

Brandeis University  
*Recapturing the Conceptual Core of General Chemistry*



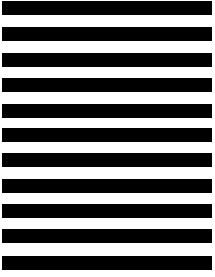
## Visitors are welcome

All seminars are held in the Pearson Chemistry Building, 62 Talbot Avenue in Medford, Room 106 at 4:30 p.m. unless otherwise noted. Refreshments are served in Pearson 102 thirty minutes prior to the seminar. For more information please contact 617-627-2634

*Newsletter*  
Department of Chemistry  
Tufts University  
62 Talbot Avenue  
Medford, MA 02155

Postage will be paid by addressee

**BUSINESS REPLY MAIL**  
FIRST CLASS MAIL PERMIT NO. 3696 BOSTON, MA



NO POSTAGE  
NECESSARY  
IF MAILED  
IN THE  
UNITED STATES



# Alumni Reply Form

Name \_\_\_\_\_

University \_\_\_\_\_

University \_\_\_\_\_

University \_\_\_\_\_

Residence Address \_\_\_\_\_

City, State, Zip \_\_\_\_\_

Firm \_\_\_\_\_

Business Address \_\_\_\_\_

City, State, Zip \_\_\_\_\_

This is a new address

Please complete and return this form for our alumni files. Include news of your current activities or suggestions for the next newsletter.

DegreeYear Adviser \_\_\_\_\_

DegreeYear Adviser \_\_\_\_\_

DegreeYear Adviser \_\_\_\_\_

Home phone \_\_\_\_\_

Position \_\_\_\_\_

Business phone \_\_\_\_\_

Name of spouse \_\_\_\_\_

I do NOT wish to have this information in the newsletter.  
(Unless you request otherwise, we will feel free to mention any of this in future newsletters.)

*Please fold here and tape shut with business reply side facing out.*

---

## INFORMATION ABOUT YOURSELF:

*cut on dotted line*

# TUFTS

TUFTS UNIVERSITY

## ChemNotes

Department of Chemistry

62 Talbot Avenue

Medford, MA 02155

---

NONPROFIT  
ORGANIZATION  
U.S. POSTAGE  
**PAID**  
BOSTON, MA  
PERMIT NO. 1161

---