Education and Research

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

RESEARCH
Elena Rybak-Akimova

The research program in the Rybak-Akimova group is aimed at designing highly specific oxidation-reduction reagents and catalysts containing transition metal ions. The significance of this research area is determined both by the fundamental problems in enzyme mimicking, and by growing industrial demand. Chemists need to be able to modify a given molecule in a specific place and to obtain a pure target product without producing many undesirable byproducts and generating harmful wastes. The group focuses on two approaches to the problem of selectivity in substrate binding and transformations: (1) introducing specific substrate binding sites into transition metal platforms; (2) investigating the detailed mechanisms of small molecule activation at the metal centers in the search for selective reactions. The research projects encompass the fields of coordination chemistry, bioinorganic chemistry, and supramolecular chemistry. The potential applications of research results include design of new selective reagents and catalysts, design of selective receptors for sensors and separation processes, drug design, and design of new materials via self-assembly and self-organization.

In order to accomplish selectivity in substrate binding, the group is designing metal-containing functional molecular tweezers, which can be opened and closed just like their mechanical counterparts. Two recognition sites are being attached to a cleft-like scaffold, so that the orientation of these receptor "arms" determines the shape of the guest which fits inside the binding site. Continued on page 2
Chemists need to be able to modify a given molecule in a specific place and to obtain a pure target product without producing many undesirable byproducts and generating harmful wastes.

length and shape are strongly bound by the newly designed molecular tweezers. The next challenges include expanding the range of the substrates, switching between binding and non-binding conformations of the tweezers, and exploring catalytic shape-selective redox reactions.

While receptor sites in molecular tweezers are responsible for selectivity in substrate binding, the metal centers are reactive and responsible for selective, site-specific transformations of the substrate. In particular, metal ions can activate dioxygen and promote selective oxidations. Oxygen is an ideal reagent for chemical oxidations, because it is readily available (air contains about 20% of oxygen) and environmentally clean (the only byproduct of the reactions is water). Oxygen is used in nature in a variety of selective chemical reactions occurring every moment in every aerobic organism, including humans. Chemists are, however, far behind nature in their ability to use oxygen for the syntheses of complicated molecules. It is easy to activate oxygen under harsh conditions, when it quickly and completely reacts with almost any organic compound, primarily producing carbon dioxide and water. This process is very useful in producing energy via burning fuels, but is not applicable to selective syntheses of desired organic products. Selective oxygen activation under mild conditions is a challenging problem. Nature uses very special catalysts, metal-containing enzymes, for selective activation of atmospheric oxygen. A general approach to oxygen activation is based on mimicking the important structural features of metalloenzymes, using small and relatively simple metal complexes. The Rybak-Akimova group is designing new macrocyclic complexes of iron for oxygen activation, and is investigating detailed mechanisms of oxygen activation. The main challenge is to suppress the production of free hydroxyl radicals that are highly active, but non-selective oxidants. In contrast, metal-based oxidants (high valent iron complexes) are much more selective. This is why an understanding of mechanistic differences between free-radical and “radical free” activation is important for revealing the mechanisms of enzyme function and for catalyst design. One might expect that mechanistic studies of oxygen and peroxide activation at the model complexes would be particularly revealing. How are peroxo intermediates formed in both mononuclear and dinuclear model complexes? How are the high-valent diamond core species formed in dinuclear systems? Are they reactive intermediates, or just the spectroscopically observable, relatively stable species? How can the O₂ molecule be activated by the model complexes, producing reactive intermediates? In order to obtain the answers relevant to rapid catalytic reactions, the individual reaction steps (formation of the intermediate from the iron complex and the oxidant, and the interaction between the intermediate and the substrate) should also be rapid. Thus, multi-mixing, stopped-flow technique is applicable to the systems of interest, and low temperatures help uncover the details of formation and reactivity of short-lived, unstable intermediates. The group is capable of performing unique experiments, where iron-based intermediates are formed at -80°C on a millisecond time scale, and then the substrates are added to the mixing cell. The most recent results show that in many cases, two irons are better than one: it is important to have two iron centers in one complex in order to achieve high reactivity of the metal-containing intermediates. Moreover, detailed mechanistic studies show that one of these iron centers is needed for oxygen coordination, while another metal binds the substrate. The results, obtained in collaboration with Prof. L. Que, Jr., and Prof. W. Tolman (University of Minnesota), open new ways for rational design of oxygen activation metallocomplexes.

EDUCATION

The Chemistry Outreach Program

Each year, Tufts University students who are enrolled in the Organic Chemistry course have an opportunity to participate in a Chemistry Outreach Program for local elementary school-age children. Professor David Walt started the program ten years ago after he presented a series of chemistry demonstrations to students at the elementary school his children attended. Both teachers and students were
captivated by the demonstrations and invited him for return visits. When he realized how much interest there was in the demonstrations, he organized an Outreach Program through the Tufts University Chemistry Department.

Typically, undergraduate chemistry and biochemistry students in their fourth semester have completed General Chemistry and are in their second semester of Organic Chemistry. These students have a very strong foundation in chemistry and are well prepared for an outreach program. When the program was initiated, the Organic Chemistry students developed a series of chemistry demonstrations that fit specific criteria:

- Supplies and equipment must transport safely.
- The volume of chemicals must be small enough to allow demonstrations to be performed in a small area but large enough so that a class of 30 students can easily see the presentation.
- Each presentation must be both educational and interesting for the age group.
- The final chemical solutions must be 'green' so they may be discarded into the sink or safely transported back to Tufts University for disposal.

The demonstrations vary from time to time but are geared to excite the students with a visual impact. Some typical demonstrations include preparing slime using polyvinyl alcohol and sodium borate, generating large quantities of foam using sodium carbonate and aluminum sulfate, observing an oscillating reaction, freezing a flower with liquid nitrogen, a chemiluminescence reaction (firefly), and generating a wide range of colors as dry ice is added to a basic solution containing a universal pH indicator. The favorite that is always included is the combustion of methanol using a miniature cannon. Most of the experiments are variations of experiments from the well-known four-volume set of chemistry demonstration by Professor Bassam Shakhashiri from University of Wisconsin.

The Outreach Program, currently under the direction of Dr. Sarah Iacobucci, director of undergraduate laboratories, has been a success for everyone involved in the program. The college students enjoy practicing and preparing for the demonstrations and are truly delighted with the reaction from young children. They return from the schools exhilarated by the experience of teaching and impressed with the intelligent

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comments and questions from the students. There is positive feedback from the children who are fascinated with the chemistry demonstrations and from the teachers and school administrators who enjoy having knowledgeable, well-prepared, enthusiastic role models visit their schools. The college students are elated when they receive a packet of thank-you cards from the children with hand-drawn pictures of them presenting the demonstrations. They find the experience so rewarding that they often organize additional visits to their hometowns and to other local schools and science fairs. For the past three years, the Tufts students have organized a science booth for the annual Tufts Kids’ Day event in April.

The number of teachers who have contacted the Chemistry Department to arrange for future visits to their schools is a testament to the success of the Outreach Program.

FACULTY PROFILE

David H. Lee

In 1959, Nobel Laureate Richard Feynman delivered his classic lecture “There’s Plenty of Room at the Bottom,” where he dreamed of fabricating materials and devices at the atomic/molecular level. At one point he said, “… The biological example of writing information on a small scale has inspired me to think of something that should be possible. Biology is not simply writing information; it is doing something about it. A biological system can be exceedingly small. Many of the cells are very tiny, but they are very active; they manufacture various substances; they walk around; they wiggle; and they do all kinds of marvelous things—all on a very small scale. Also, they store information. Consider the possibility that we too can make a thing very small which does what we want—that we can manufacture an object that maneuvers at that level!” This convergence of biology with molecular design and chemistry at the intersection of nanotechnology underlies the research program of David Lee, our newest faculty member.

Dr. Lee’s background makes him ideally suited for this endeavor. His undergraduate research experience included work in labs focusing on physical organic chemistry, structural biology, and pharmacology. He thought however, that he was bound for medical school until he visited the Scripps Research Institute. When he saw how labs there were effectively combining organic chemistry, structural and cell biology into imaginative research programs that tackled challenging problems in biomedicine, he was hooked. “I would have wondered for the rest of my life what I would have missed if I didn’t go,” he remarked. He obtained a Ph.D. there in Reza Ghadiri’s lab after designing and characterizing the first self-replicating peptide, a feat which caught the attention of those interested in the chemistry underlying the origins of life. “Nucleic acids are the traditional vessels of information necessary for reproduction in an organism,” he explained, “Peptides and protein contain information too but it is much more complex to understand because of its three-dimensional aspect. In this case however, we were able to harness it.” He then moved to the east coast and did postdoctoral work in Peter Kim’s lab at the Whitehead Institute for Biomedical Research at MIT where he used his experience in molecular design to address the question of how the AIDS virus enters a cell. While there, he also carried out biophysical studies on Acrp30, a self-assembling protein hormone that holds great promise for treating chronic obesity and insulin resistance.

What does Dr. Lee have planned now that he’s arrived at Tufts? This brings us to Feynman’s lecture. “I would love to build functional nanoscale devices!” he exclaimed, “The field of nanotechnology, however, is still in its infancy. One great bottleneck is that we still don’t know many of the fundamental properties of nanoscale–organized molecules and quantum dots. This is because we are still novices at building sophisticated supramolecular structures. Biology however, has come up with efficient bottom-up approaches to build them by self-assembly, from viruses to the cytoskeleton and beyond! I think this is where my experience in molecular biology and in designing self-assembling proteins can have a big impact on how we explore nanoscale chemical systems. For instance, I’d like to use biological systems to organize quantum dots and self-assemble them into novel structures. Perhaps then, we can gain insight into their chemistry and get a firm footing for the rational design of molecular devices. I can’t wait to start because the diverse and intellectually rich atmosphere of Tufts Chemistry makes it a great department in which to do such multidisciplinary research.”
### Undergraduates

#### Chemistry Major

**Awards Presented 2001-2002**

- **The R.M. Karapetoff Cobb Award**
  - Brooke Nussbaum
  - Devon Snow

- **The M.D. Angell & H.B. Durkee Scholarship**
  - Tanya Gustafson

- **The Durkee Scholarship**
  - Pascal Dabel
  - Millicent Smith

- **The Max Tishler Prize Scholarship**
  - Brooke Nussbaum
  - Philip Vitorino

- **The Thomas Harrison Carmichael and Emily Leonard Carmichael Prize Scholarship**
  - Philip Vitorino

- **The Marshall Hochhauser Prize**
  - Bradley Crotty

- **The Benjamin G. Brown Scholarship**
  - Tanya Gustafson

- **The Class of 1947 Victor Prather Prize**
  - Bradley Crotty
  - Tanya Gustafson

- **Summa cum laude**
  - Tanya Gustafson
  - Nichole Bosson

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### Bachelor's Degrees Awarded 2002

- Philipp Anwer
- Nicole Bosson
- Emily Briggs
- Pascal Dabel
- Sarah Gardner
- Tanya Gustafson
- Mark Kristjanson
- Jodie Moreau
- Douglas Rosenberg
- Millicent Smith

### Rosemary Feeney

(Kounaves) "Development, Demonstration, and Validation of Microfabricated Iridium and Gold Arrays for the Field Screening of Heavy Metals in Ground Water"

### William Connors

(Richert) "Enforcing DNA Duplexes with Molecular Caps"

### Kendra Dombi

(Richert) "New Methods for Generating and Studying Modified Oligonucleotides and Porphyrins"

### Master's Degrees Awarded 2001-2002

- Michael Fleming
- Kristin Gordon
- Janet Herdan

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### CGSC News

The Chemistry Graduate Student Council (CGSC) originated to increase communication between graduate students, faculty, and staff and to promote a positive academic and working environment for graduate students in the chemistry department. During its first year, the CGSC had numerous accomplishments: alleviating some of the mysteries behind study topics by creating a database of previous study topics; gathering graduate student input on faculty candidates; helping to organize Spring Graduate Open House; mentoring incoming graduate students. The CGSC worked diligently to help assess the needs of graduate students with the participation of the entire department.

Last spring, the CGSC held its first official election. The graduate students and the five elected officials, Brian Corneau, Jenny Tam, Irene Li, Kevin Clow, and Sandra Bencic celebrated this monumental event with a rockin' BBQ courtesy of Kate Myers and her roommates. Each student represents a class year and continues the work set in motion from the previous year.

The CGSC recently filed a constitution and is now a recognized body of the GSC – the university-wide Graduate Student Council – complete with its own budget and voting power on the GSC. Sandra Bencic and Adam Carberry work with the GSC, to keep the chemistry department active in the graduate school. Dan Killelea organizes graduate student seminars once a month so that students can learn about other research in the department. These seminars also provide a forum for fresh ideas.

Not to worry — the CGSC isn't all work and no play. The softball team, the Isotopes, finished the season with a .500 record. The fall semester began with a whitewater-rafting trip on the Penobscot River in Maine. Every Wednesday, the volleyball team represents the department on the court. On alternate Fridays, when there isn't a flag football game, graduate students meet at Café Chem for a social gathering.

The momentum of the CGSC continues to grow. The CGSC will continue to address important topics and generate new ideas.
Marc d’Alarcao received the Lillian and Joseph Leibner Award for distinguished teaching and advising.

“Quality of Life,” a documentary film produced by Michelle DeBakey, former staff assistant in Chemistry, was shown at the New York Independent Film and Video Festival.

Bob Dewald offered a Glass Blowing Demonstration and Lecture during the spring semester in response to requests from the Tufts Undergraduate ACS chapter.

Sarah Iacobucci, director of Chemistry Undergraduate Laboratories, continues to be active in the Northeast Chapter of the American Chemical Society (ACS). The chapter’s Education Committee was given a ChemLuminary award for Outstanding Performance by a Large Size Local Section during 2001. The National Chemistry Week events reached an audience of about 6,000.

Jonathan Kenny has been appointed director of the Center for Interdisciplinary Studies for the next three years.

The university selection committee for the PEW Scholars Program selected Dave Lee’s proposal to represent Tufts for the Biomedical Sciences Award.

The Chemistry Department celebrated Bob Stolow’s 70th birthday with a reception at the Remis Sculpture Court at the Aidekman Art Center.

### Semester Achievement Awards

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<td>Debbie D’Andrea</td>
<td>Dave Wilbur</td>
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<td>Kerin Clow</td>
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Scenes from the summer graduate student picnic.
Our graduate students continue to set a high standard for achievement. For the second year in a row, the graduate school Outstanding Achievement Award went to a chemistry graduate student. This award was given to Nicholas Yoder in recognition of contributions to undergraduate education as well as individual academic achievement. Congratulations to both Tanya and Nicholas!

Our new faculty member, David Lee, comes to us from the Whitehead Institute for Biomedical Research in Cambridge. His research is in the biochemical area, starting with projects on biomineralization and fibrous proteins. Professor Lee has a real passion for his science and unbounded enthusiasm and energy. Welcome aboard Professor Lee!

You are all invited to stop by the department and see the newly renovated main lecture hall – you will be amazed at the transformation. Site lines have been improved by angling boards and seating, a state-of-the-art projection and sound system has been installed and, of particular interest to any of you who were in that room on those very warm days, the room is now fully climate controlled. The lecture room has not yet been named, so an opportunity exists for anyone interested.

In other news, the department celebrated the 70th birthday of Professor Robert Stolow. Professor Stolow’s former students came from near and far to help the department celebrate this milestone. Later in the spring, the faculty set aside a half day to engage in our first retreat to kick off a self-evaluation and direction-setting mission. There was unanimous agreement that our most pressing need is for upgrading and renovating the facilities. We will be looking to friends of the department for help in accomplishing this goal.

Stay tuned for further developments.

Your former teachers and colleagues would like to hear about you. Send your updates to arlene.chaplin@tufts.edu so you can be included in Class Notes.
Class Notes

Steve Baldelli (1998) gave an invited presentation at the FACSS (Federation of Analytical Chemistry Societies) meeting in Providence, RI in October. Steve is currently an assistant professor at the University of Houston doing research focusing on ionic liquids – prime candidates for “green chemistry.”

Alex Kornienko (1999) completed two years of postdoctoral research at the University of Montreal, working on design and synthesis of new antibiotics to be used to treat bacterial infections, characteristic for children with cystic fibrosis. In the Fall of 2002, he joined the Department of Chemistry at New Mexico Tech as an assistant professor where he teaches freshman and Organic Chemistry classes as well as upper division courses, such as Advanced Organic Synthesis, Organo-metallic and Medicinal Chemistry. He supervises a research group that is working on a variety of projects involving chemical synthesis of anticancer agents and developing new molecular electronic devices and artificial photosynthetic molecular systems.

Georgia Marnera (2001) is currently working at Arriani Pharmaceuticals in Greece, where she is a junior product manager responsible for the dental line of products.

Peter A. Peterson (1947), professor of Plant Genetics at Iowa State University, is teaching a course on the history or development of hereditary concepts beginning in the pre-literate era through the modern era of molecular biology. He continues his research in genetics.

Cheryl Schnitzer (1999), assistant professor of Chemistry at Stonehill College, established Project SEED (Summer Educational Experience for the Disadvantaged), a program designed to encourage careers in chemical sciences. In this program, high school students conduct paid research alongside Stonehill faculty.

The Tufts Chemistry WEB site!

http://chem.tufts.edu

Our 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 (Samuel.Kounaves<at>tufts.edu).

IN MEMORIAM

Friends and classmates of the late CARYL BOYDEN (1950) made donations to the Chemistry Department in her memory. She touched many lives and was an inspiration to many.

MATTHEW L. HERZ died on November 11, 2000. He received a doctorate from University of Rhode Island and an M.B.A. from Boston University. He was chief scientist at the U.S. Army Laboratory in Natick, MA and was awarded the Meritorious Civilian Service Award and Medal.

EDWARD KOSTINER, (1960) emeritus professor of Chemistry at University of Connecticut died on February 10, 2002. He received a Ph.D. from Polytechnic University of Brooklyn.

DON WILEY, (1966), professor of biochemistry at Harvard University, died in December 2001. He served on the Chemistry Department Advisory Board. His research focused on molecular mechanisms that enable viruses to infect cells. he was the recipient of many prestigious awards including the Albert Lasker Medical Research Award and the Japan Prize from the Science and Technology Foundation of Japan, which he shared with colleague, Jack Strominger.

KENT WILSON, former chair of the Tufts Chemistry Department and long time NSF administrator, died in December, 2000. He is survived by his wife, Gladys Wilson, and his son, Matthew.
Seminar Series

JANUARY 21
Prof. William Reiff
Northeastern University
On the Complex Magnetism of Seemingly Simple Dimers: From Disappearing Hyperfine Effects to Cooperative Long Range Order to Quantum Tunneling of Magnetization

JANUARY 28
Prof. Stephen Lippard
Massachusetts Institute of Technology
Non-Heme Iron and the Biological Oxidation of Methane

FEBRUARY 4
Prof. Christopher Arumainayagam
Wellesley College
Electron-Induced Reactions in Nanoscale Thin Films

FEBRUARY 11
Prof. James McKnight
Boston University
Cross-Examining a Villin: Structure, Function and Folding of a Small F-Actin-binding Domain

FEBRUARY 18
Prof. Linda McGown
Duke University
DNA Aptamers in Proteomic Analysis

FEBRUARY 25
Dr. Russell Petter
Biogen, Inc.
Remarkably Potent Antagonists of Integrin VLA-4

MARCH 4
Prof. Barry Karger
Northeastern University
New Technologies for Genomics and Proteomics Based on High Resolution Electrophoresis and Chromatography

MARCH 13
Prof. Robert Walker
University of Maryland
Solvation at Surfaces: Profiling Interfacial Solvent Polarity with Molecular Rulers

APRIL 1
Prof. Chaitan Khosla
Stanford University
Chemistry and Biology of Celiac Sprue

APRIL 15
Prof. Heidi Martin
Case Western Reserve University
Diamond-based Electrodes as Neurochemical Sensors

APRIL 22
Prof. Hicham Fenniri
Purdue University
Rosette Nanotubes: New Materials with Unprecedented Properties

MAY 13
Prof. Allen J. Bard
University of Texas, Austin
Application of Scanning Electrochemical Microscopy in High Resolution Investigation of Interfaces.

Visitors are welcome
All seminars are held in the Pearson Chemistry Building, 62 Talbot Avenue in Medford, Room P-106 at 4:30 p.m. unless otherwise noted. Refreshments served in Pearson 102 thirty minutes prior to the seminar. For more information please contact Janice Silva at 617-627-2634 or anice.silva@tufts.edu.
ChemNotes

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