

The Carnegie Mellon Chemist

CHEMISTRY DEPARTMENT NEWSLETTER



CARNEGIE MELLON UNIVERSITY

January 2001

No. 11

Chemistry Undergrads

2000 Graduating Class

The 2000 Carnegie Mellon Commencement included 23 Chemistry majors, 19 BS and 4 BA. One of these graduates, Michael O'Kelly, earned three separate BS degrees, one each in Chemistry, Physics, and Mathematical Sciences (this may be a first—anyone know of a precedent?). He was also the recipient of a Hertz Fellowship and is now attending graduate school at California Institute of Technology. Sixteen students are attending graduate school, one is in medical school, five have industrial positions, and one is a 2nd Lieutenant in the army. Eight received Senior Leadership Awards, eight received University Honors, eleven received College Honors, and three received Departmental Honors. Two each were inducted into Phi Beta Kappa and Phi Kappa Phi. Graduate schools our majors are attending are: Stanford, Berkeley, Princeton, MIT, University of Wisconsin, University of North Carolina, SUNY, University of Illinois, Northwestern, University of Florida, University of Washington, University of California-Santa Barbara, Case Western, Carnegie Mellon - Heinz School. Positions were also

Continued on p. 3 ☞

Teacher-Scholar Award

David Yaron has received a *Henry Dreyfus Teacher-Scholar Award*.

Like other Dreyfus Foundation awards, this award is given to faculty relatively early in their careers who excel in both academic research and teaching. The *Henry Dreyfus Teacher-Scholar Award* emphasizes the nominee's accomplishments in research, teaching and mentorship, particularly with undergraduates. Dave's models for the photophysical and electronic properties of conjugated polymers are designed to establish structure-property relationships in these materials with applications in, for example, flat screen displays, organic transistors, and photocells. The unique aspects of his model are the inclusion of dielectric interactions between chains in the solid state, and the use of an effective particle approach, adapted from solid-state physics, to make calculations on long polymer chains computationally feasible. Professor Yaron also leads a group developing innovative educational software for introductory chemistry courses.

This project has produced a highly flexible Virtual Laboratory and is now producing authoring tools and components to make it possible for

Continued on p. 5 ☞

Truman Kohman Honored

Truman Kohman, Emeritus Chemistry Professor, has been honored by the International Astronomical Union (IAU), the organization in charge of naming new celestial bodies. A minor planet discovered in 1987 by astronomer Edward Bowell at the Anderson Mesa Station of the Lowell Observatory in Arizona has been named 4177-Kohman by the IAU. Truman was nominated for the honor by Bruce Hapke and William Cassidy, professors of geology and planetary science at the University of Pittsburgh. They cited his discovery of the aluminum-26 nuclide as giving astronomers important information about meteorites and the early history of the solar system. Truman said he was "surprised and delighted" to have an asteroid named after him. He describes 4177-Kohman as a typical main-belt asteroid orbiting the Sun, between the orbits of Mars and Jupiter once every 6.02 years. His namesake, estimated to be between 15-30 kilometers in diameter, probably comprises carbon-based matter. Only two others associated with CMU have minor planets named after them: Andrew Carnegie, our

Continued on p. 5 ☞



The Department Head's Column

It is my pleasure to update you on recent achievements in the Department: three new outstanding faculty members hired; approval to build new undergraduate teaching laboratories secured; the requirements for graduate studies improved; and the recruitment of graduate students greatly expanded. You will read more about these accomplishments elsewhere in this issue.

Tomasz Kowalewski joins us from Washington University in St. Louis as a physical polymer chemist, Neil Donahue, an atmospheric chemist from Harvard, has been appointed jointly in Chemistry and Chemical Engineering, and bioinorganic chemist Catalina Achim will join us from Harvard in the Fall of 2001. Work by Terry Collins' group that earned the 1999 Presidential Green Chemistry Challenge Award was further recognized when he was one of only three award winners featured in a Green Chemistry video produced by the ACS and EPA. Dave Yaron has received the very prestigious *Henry Dreyfus Teacher Scholar Award* for his outstanding scientific accomplishments and dedication to undergraduate education. (Terry Collins won the same award 15 years ago.)

Our research and educational funding has expanded and taken some exciting new directions. For example, Bruce Armitage has received major support from both NSF and NIH for his PNA work, including a collaboration with Guy Berry and Gary Patterson to study reversible polymer gels. Mike Hendrich's cutting edge work on metal clusters in proteins continues to receive excellent support from the NIH and has appeared in C&E News; Mike was recently awarded (indefinite tenure). In addition, we have grown nearly \$1 million in our funding for educational activities. Dave Yaron and Rea Freeland received a grant, in collaboration with computer scientists at Brown University, to develop educational software and authoring tools for the NSF's Digital Library project. Karen Stump has secured a large three-year grant from the Pennsylvania Department of Education to conduct the Governor's Institute for Physical Science Educators.

As always, we take great pride in the excellence of our graduates. The Class of 2000 was extremely active in research. The majority of the class went on to outstanding PhD programs or accepted excellent industrial positions. We are also excited that we granted twelve doctoral degrees this May. Of these new PhD's, one now has a tenure track position at Allegheny College, four have post doctoral fellowships in outstanding groups at Yale, NC State, University of Minnesota, and NIST, and several others have industrial positions such as at Magellan and Bayer. We look forward to more of this success for our current students.

The near future promises further growth and excitement for the department. We are currently searching for additional new faculty in organic chemistry and theoretical/computational chemistry. I am also pleased to announce that the Board of Trustees have approved the \$23M undergraduate chemistry teaching laboratories, and that the project is now underway. These and other changes lay an even stronger foundation for the excellence you expect in the Department.

Richard D. McCullough

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Faculty Profiles

This issue profiles one of our veterans, and two of our new members:

Linda A. Peteanu

was promoted to Associate Professor last year. Linda joined the department as an Assistant Professor in Spring 1993. Research programs in her group span materials science, photochemistry, and biology. Work thus far has been concerned with measurements of the basic electronic properties of molecules that have photo-chemical and/or photo-biological importance, and with comparison of the results of measurements to the predictions of electronic structure theory. These comparisons are designed to elucidate the intrinsic properties of these systems as well as

Continued on p. 6

Neil Donahue

joined the department as an Assistant Professor in the fall of 2000, coming to CMU from Harvard with a joint appointment in Chemistry and Chemical Engineering. His career has been quintessentially interdisciplinary; he has an AB in physics from Brown University, a PhD in meteorology from MIT, and pursued a post-doc in gas-phase physical chemistry at Harvard, where he remained for nine years as director of the atmospheric kinetics program in Jim Anderson's research group. Neil has a broad set of research interests, ranging from theoretical studies of chemical reactivity to in-situ measurement of free radicals in the atmosphere. However, the common

Continued on p. 6

Tomasz (Tomek) Kowalewski

joined the Chemistry Department in August 2000 as Assistant Professor, coming from the Department of Chemistry at Washington University in St. Louis, where he was a Research Assistant Professor. His research is on the physical chemistry of macromolecules and soft condensed matter, with particular emphasis on self-organization. After receiving a PhD from the Polish Academy of Sciences (Center of Molecular and Macromolecular Studies) he initially joined the group of Professor Jacob Schaefer (a CMU alumnus) in the Department of Chemistry at Washington University, and then initiated and developed an independent interdisciplinary research program, exploring the use of

Continued on p. 6

Chemistry Undergrads

Continued from page 1

obtained at DuPont Pharma, Pfizer, Bristol Myers Squibb, Environ Group, and the U.S. Patent and Trademark Office.

Recognition

Christopher Noser was one of eight students in CMU to receive a *Fifth Year Scholarship*, and Scott Vignon received an *Andrew Carnegie Society Award*. Both were selected as Beckmann Scholars for the 2000/01 academic year.

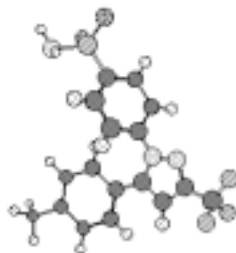
Lab Renovation

The renovation of the Chemistry Undergraduate Teaching Labs described in the last issue of these pages has begun. The renovation promises to move these important teaching labs into the 21st century, to better enable us to deliver a quality education to our students. Follow the progress on the Department's web page as we proceed: links are provided there to artistic renditions of the renovations and floor plans.

Freshman Chem Graphics

Charles H. VanDyke has arranged to have copies of CambridgeSoft's computer software ChemDraw and Chem3D included with each textbook used in the freshman chemistry course that he teaches. Structure and bonding principles have been a major part of 09-105 for many years. Exercises were given in which students could generate professionally drawn structure representations and chemical equations, and also examine various structural features of the molecules. Initially, the structure exercises involved determining bond length and bond angle parameters for simple organic molecules containing single, double, and triple bonds. Data for benzene illustrated resonance effects. Some background in organic chemistry was provided, and students became familiar with line-drawn representations of organic compounds. Students were then asked to predict the structural features of a variety of more complex molecules, and compare their predictions with data generated by the

Chem3D program or as provided by structures elsewhere (e.g. www.webmolecules.com). Exercises ranged from comparing the structure of menthol with its aromatic equivalent thymol, to examining the structures of methylisocyanate, nicotine, tetrahydrocannabinol and the stereocenters in ibuprofen and thalidomide. Structural features of the new "superaspirin" compounds Vioxx and Celebrex were examined. Examining the structure of buckminsterfullerene, C₆₀, generated a lot of enthusiasm and the students could rotate and observe the 20 hexagonal and 12 pentagonal faces of the molecule and determine that one of the three bond angles at each carbon center was distorted from the usual sp² 120° angle to 108°. Some work with polymers was included, including representations of organic conducting polymers (e.g. cis and trans forms of polyacetylene), and examining the structures of atactic, isotactic and syndiotactic forms of polypropylene. Initially, many of the structural determination exercises were done on a discovery basis without providing much background in bonding theory. Concepts of hybrid and molecular orbitals were covered in detail and related to the structure exercises as the course progressed. Hopefully by the end of the course, students had a more complete appreciation for why compounds have their structures, and where appropriate, how some of the observed properties of the compounds can be related to molecular structure.



A model of Celebrex

Organic Chemistry

Bruce Armitage, an Assistant Professor who teaches Organic II, recognizes that organic chemistry is an intimidating sub-

ject for most students. Multistep synthesis, reaction mechanisms, and spectroscopic structure determination are all topics that challenge students, and Organic Chemistry lecture courses at 8:30 AM only add to the difficulty in drawing students into the subject. According to Armitage, "The reputation and meeting time are like having two strikes on you before you even get to the plate. You have to get the students' attention and gain their confidence very early in the semester, or else they'll tune out. Nearly every student in the class is taking it either to fulfill a degree requirement or to prepare for the MCAT. That doesn't mean they are a captive audience, though. It's awfully easy to sleep through an 8:30 AM class, especially if you don't think attending the class will help your performance." In order to get the students interested in the topic, applications of organic chemistry to other fields are emphasized, such as the biological sciences, medicine and materials sciences. After the first 10 weeks of the semester devoted to classical organic chemistry topics, Armitage broadens his subjects to include a week of lectures on polymer chemistry, two weeks on proteins and nucleic acids ("bioorganic chemistry"), and a lecture on the organic chemistry of narcotics, to spark the interest of even the most reluctant student. He credits the possibility of this broad approach to the solid foundation the students receive in the first semester of the sequence with Professor Stu Staley: "Stu gives the students their first introduction to all of the most difficult topics ranging from stereochemistry to synthesis. I get the easy stuff." Gaining the students' confidence is another issue, especially since Armitage uses pop quizzes to gauge student learning and encourage attendance, and does not use a curve for the class. "That really scares a lot of the students, but I have fairly liberal policies for dropping homework, quiz and even exam scores. The benefit to the student is that they can calculate their standing in the class at any time. I just have to reassure

them that I can write an exam that gives them a fair chance of getting an A." Otherwise, Armitage focuses on engaging the students in the material "I try to make my enthusiasm for Organic obvious to the students. Seeing that some people actually enjoy this stuff helps minimize the intimidation factor." Armitage also tells the Monday Morning Joke to help lighten things up – "I can't guarantee they'll laugh each week, but the students seem to appreciate the effort"--and relates many of his own experiences as an organic chemistry student, which he refers to as the "I-feel-your-pain approach". Overall, the efforts seem to be paying off as the students in Organic II have given the course overall ratings of 4.65 (Spring 1999) and 4.82 (Spring 2000) out of 5. The real test, though, comes with the students who go on to take the MCAT or GRE exams. "If they do well on the organic chemistry sections of those exams, then I feel like we did a good job of preparing them", says Armitage.

Off-Campus Activities

Scott Vignon spent the summer at Umea University in Sweden, working on a research project on ring inversion supervised by Stu Staley. Three chemistry undergrads are in the Studies Abroad program this year: Evan Beach (New Zealand), Naima Hall (EPFL) and Kris Stokes (Denmark). Kris sent us the following comments on his experience: "I got to Denmark in June. Within a week of being here, I began an intensive language program in order to learn the Danish language. It was a class for 3 hours per day, 5 days per week, and over a total of 8 weeks. After my class, I went to the lab to work on polythiophene synthesis of all kinds for Thomas Bjornholm, one of Prof. McCullough's collaborators. Once the fall arrived, I enrolled in a class called "The Physics and Chemistry of Nanostructures" as well as continuing my labwork. My time here has not been entirely work related, though. Last summer, I took a two week trip through Germany and the Czech Republic, as well as a week at the beginning of

December to visit a former post-doc from the McCullough lab at her home in France, where I was exposed to escargot, frog legs, and fuzzy cheeses. Spending a semester in Denmark has been an excellent experience for me, not so much for the chemistry that I have learned while working, but more so for the many different people I have met both inside and outside the lab. However, I am also very excited to come back to Pittsburgh, and finish up my studies there in the spring."

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Outreach Activities

Karen Stump was the On-Site Director for the second Pennsylvania Governor's Institute for Physical Science Educators (GIPSE), hosted by Carnegie Mellon, July 9-21, 2000. The Institute is one of over 20 Governor's Institutes and Academies offered for the professional development of Pennsylvania K-12 teachers, funded by a Pennsylvania Department of Education grant. This past summer 24 teachers (3 elementary, 11 middle school and 10 high school) participated in a curriculum focused on 5 thematic areas: astrophysics, materials, biopolymers, chemicals and particle physics. The faculty were a mix of K-12 teachers and faculty from the Mellon College of Science at CMU. Participants from the chemistry department included Rick McCullough who gave one of 5 keynote addresses, Dave Yaron who spoke with a group of teachers about Project Irydium, and Hugh Carr, John Ziegler and Mark Stauffer who offered a series of workshops drawn from their work with the CMU Van Program. The third Institute will run July 8-20, 2001.

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Graduate Program

Chemistry graduate students Nadine Fattaleh-Diggs won the *Hugh D. Young Graduate Student Teaching Award* for 2000. In the five years that this award has been given, Nadine is the fourth chemistry graduate student to be so honored. She was

cited for having a significant impact on an unusually broad set of courses during her tenure as a TA, including freshman chemistry, organic and inorganic, and the laboratory program. Kathryn Beers and Marion Gehrman won the Chemistry Department Graduate Teaching Awards for 2000. Nadine Fattaleh-Diggs, Missy Pasquinelli, and Dan Savin are Teaching Fellows in the Eberly Center for Teaching Excellence.

Throughout this year the Department has devoted substantial attention to enhancing the graduate program, both in recruiting and in improving the experience of our current students. **Eckard Münck**, as Chair of Graduate Admissions and Recruiting, is establishing relationships with many of the outstanding four year colleges in our region as well as excellent schools internationally. By working with faculty at schools like Hamilton, Juniata, and Washington and Lee, we are establishing "pipelines" to attract a few students from those programs to Carnegie Mellon on a regular basis. This year's entering class includes students from Allegheny College and the University of Bucharest who were recruited in this way and we look forward to more in the future.

With extensive student input, the department has also developed a plan to increase students' momentum on their research and feedback from advisors, advisory committee members, and the department as a whole. Specific changes include: a more in-depth focus on the research progress report, an original proposal that may be in the student's general research area, annual advisory committee meetings that help ABD students focus on dissertation planning, and an annual review of student progress.

Information on the graduate program is available on the department web site. We encourage you to help prospective students learn more about us.

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Teacher-Scholar Award

(continued from page 1)

instructors with minimal programming skill to create their own on-line learning activities. In addition, Dave has contributed substantially to the departmental curriculum by creating a hands-on computational chemistry course, adding numerous innovations to Modern Chemistry II, and securing both computers and fellowships to support computational chemistry students. The *Henry Dreyfus Teacher-Scholar Award* was awarded to five individuals this year--Dave is the only recipient at a research university.

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Truman Kohman Honored

(continued from page 1)

founder, and John Brashear, a distinguished astronomer and director of the Allegheny Observatory who was part of the first faculty of the Carnegie Institute of Technology--Kohman nominated Brashear for that honor. Truman, who taught nuclear chemistry, is an avid amateur astronomer whose interests led him to teach an introductory astronomy course at Carnegie Mellon for 20 years, including nine years after his formal retirement in 1981. He is a long-time member of Amateur Astronomers Association of Pittsburgh and was recently elected to honorary membership.

Truman has published a biographical memoir of John (Jake) C. Warner in volume 78 of *Biographical Memoirs*, published by the National Academy Press, Washington, D.C. A copy may be read at the url: books.nap.edu/books/030907035X/html/318.html#pagetop

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Librarian Moves On

Lynn A. Labun, who helped many a bewildered user deal with the mysteries of searching the Library at Mellon Institute for information on-line or the "old fashioned" way, on-shelf, has moved on to a new phase of her career. Lynn started as an Information Assistant at Hunt Library, while pursuing a Masters

of Library Science from the University of Pittsburgh. After receiving that degree in 1982, and a stint at the Engineering and Science Library, she was named to head the Mellon Institute Library in 1986. While helping that facility modernize to the fine service it is today, she earned a Master of Public Policy and Management from CMU's Heinz School. So armed, she has become a research analyst in the Office of Development, charged to identify foundations that might be interested in supporting the university, using her library skills in background research on prospects.

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A Staff Profile

Drew Potratz joined the department in July 2000 from Computing Services to become our Senior Systems/Software Engineer. Drew has a BS in Mathematics/Computer Science from Carnegie Mellon and more than 10 years experience with a variety of platforms. He administers file, print and computer servers as well as providing some desktop support for the faculty and the Dean's Office. In just three months, he has brought calm and expertise to tasks where faculty previously had to fend for themselves. In the coming months, Drew will work on improving our computing infrastructure with systematic backups and added security.

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Faculty Affairs

Catalina Achim will join the Chemistry Department in Fall 2001. Currently a Postdoctoral Fellow at Harvard University, Catalina earned her PhD at CMU in 1998, working under the supervision of Eckard Münck. She is interested in polynuclear clusters that are redox centers in iron-sulfur proteins, iron-oxo proteins such as methane monooxygenase and ribonucleotide reductase, and the Mn water-oxidation catalyst of photosystem II. Her studies will aim to elucidate the electronic structure of clusters and their function in biological

systems, and identify molecules with special properties.

Paul J. Karol spent his fall semester sabbatical as a Visiting Professor and Japan Science and Technology Agency Fellow at the Japan Atomic Energy Research Institute in Tokai, Japan, about 100 miles northeast of Tokyo, on Honshu's Pacific Coast. Professor Karol was involved in research on the production yields and chemistry of short-lived isotopes of the elements rutherfordium (Z=104) and dubnium (Z=105). The Tokai laboratory is one of a handful worldwide capable of producing these species. Many hours of beam time are needed to generate even a few dozen measured atoms, so the apparatus and experimental protocol are not typical of a conventional chemistry investigation. One interesting aspect of the studies is how various relativistic effects associated with rutherfordium's high Z cause departure from the trends evident in a chemical group from those that Mendeleev recognized in launching the original periodic table. In addition to the heavy element chemistry studies, Karol also discussed possible future collaborations at a new Tokai facility being proposed, to work on his long-held interest of accelerator transmutation of nuclear waste.

Linda Peteanu visited Japan, for three weeks under the auspices of the Japan Society for the Promotion of Science. Hosted at the Institute for Electronic Science at Hokkaido University, she gave lectures there and at other venues in Japan.

Guy C. Berry delivered the Plenary Lecture at ChiPol-2000, a meeting of polymer scientists in Chile in December. He elected to go to a "phased-retirement" status at the start of the 2000-01 academic year, to be half-time for the next four years.

Morton Kaplan spent his sabbatical leave at the Brookhaven National Laboratory, working on the STAR project described in the last issue of these pages. Details of the project may be found at www.star.bnl.gov.

Faculty Profiles (Continued from p. 2)

Peteanu

to show how these properties are modified by molecular interactions with glassy, polymeric, or biological matrices. The research emphasizes the use of electroabsorption (Stark) spectroscopy. This involves applying an external electric field to a molecule and analyzing the resulting shift in its absorption spectrum to determine the change in dipole moment and the change in polarizability upon photo-excitation to a higher-lying electronic state. This information is directly related to the extent of charge transfer and the degree of electron de-localization present in the excited state relative to the ground state. In the past several years, Peteanu's group has used this method to study molecules and proteins that undergo photo-induced reactions, such as charge transfer and isomerization, as well as the mobility of small molecules in polymer films, and disorder in conducting polymer systems.

Donahue

there is a desire to elucidate the underlying physical chemistry of the earth's atmosphere and to design measurements that rigorously test that chemistry. A particular objective is to understand how the complex chemical system that is the atmosphere will respond to inputs due to human activity, whether it be temperature variations due to climate change or changes in composition due to industrial emissions. Neil is excited by the opportunity to bridge two very strong programs related to environmental chemistry. In the Chemistry department, he joins the Green and Environmental Chemistry area, with strong links to groups in both physical and theoretical chemistry. He is keen to help expand the graduate and undergraduate research program in this area. Professor Donahue's laboratories are in Doherty Hall, where he joins the air quality group, including Professors Spyros Pandis (Chemical Eng. and Engineering and Public Policy), Cliff Davidson (Civil and Environmental Engineering) and Allan Robinson (Mechanical Engineering), sharing space in the new Air Quality Laboratory. This large, state of the art facility is designed to foster collaboration among the various research projects, many of them focused on the origin, chemistry and fate of organic particulates in the atmosphere. Neil and his family live in Squirrel Hill -- he bikes in daily with his daughter in tow, bound for her preschool on the campus.

Kowalewski

proximal probe techniques to study synthetic and biological macromolecules. These techniques, which are facilitating the rapidly growing field of nanoscience, directly study and manipulate matter at a scale down to individual molecules and atoms. His accomplishments included: the development and characterization of a new class of macromolecules -- shell-crosslinked nanoparticles-- in collaboration with Prof. Karen Wooley; insights into the process of DNA end-joining; and

characterization of the mechanical properties of individual carbon nanotubes, the novel form of carbon attracting attention for its potential in molecular electronics and nanocomposites. He also demonstrated that the assembly of β -amyloid peptides into toxic aggregates, one of the major "suspects" in Alzheimer's disease, can be driven by interactions with surfaces. The physical chemistry of Alzheimer's disease will remain a focus of Tomek's research at CMU, along with structural studies of glassy polymers and studies of wetting of polymer surfaces. His laboratory is also becoming a hub of collaborative pursuits between synthetic and physical chemists aimed at tailoring novel nanostructured materials through the precise control of their macromolecular composition and architecture.



Atomic Force Microscopy image of DNA-dependent protein kinase (DNA-PK) molecules bound to double-stranded DNA. Such interactions are crucial in the synthesis of antibodies and in DNA repair.

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Research Profiles

Krzysztof (Kris) Matyjaszewski has formed a new Controlled Radical Polymerization (CRP) Consortium to support research in that area in his laboratories for the next five years. The CRP Consortium succeeds and broadens the scope of the former ATRP Consortium, established in 1996 and dedicated to the study of atom transfer radical polymerization. Currently 19 companies from US, Mexico, Japan, France, Germany, Holland, Belgium, Switzerland and South Africa have joined the new CRP Consortium. Atom Transfer Radical Polymerization (ATRP) was disclosed by Professor Matyjaszewski as a new method of controlling radical polymerization in April 1995, during the presentation to him of the ACS Carl S. Marvel Award for Creative Polymer Chemistry. The participation of industrial sponsors demonstrates the great number of potential commercial applications for products based on a viable controlled radical polymerization process. The estimates of the market affected by CRP processes exceed \$20 billion/year.

Since the publication of the first paper on ATRP (Wang, J.-S.; Matyjaszewski, K. *J. Am. Chem. Soc.* 1995, 117, 5614) over 1,000 papers and patent applications devoted to ATRP have been published, with the number of publications approximately doubling each year. During the past five years the ATRP Consortium focused on three areas:

1. The mechanism of ATRP processes by determining the structure of the active reagents and the correlation of structure with reactivity.
2. Optimization of ATRP to expand the range of polymerizable monomers, initiators, and catalysts, with the objective of running ATRP under very

robust commercially viable conditions, including aqueous systems.

3. Preparation of well-defined (co)polymers with controlled topologies, compositions and functionality, allowing structure-property correlation for the synthesized materials.

The studies on ATRP have involved 25 postdoctoral fellows, 23 graduate and 26 undergraduate students. The results were published in over 200 papers and led to 7 US Patents (11 applications are pending); as well as 14 allowed international patents (with over 50 active applications). The research on ATRP and other CRP studies will be continued to reach the original goals of fundamental structure-reactivity and structure-property correlations, as well as optimization of the reaction conditions for the prepared polymeric materials to provide the technology required by Consortium Members to develop new products.



The Matyjaszewskis with Aleksander Kwasniewski, President of Poland (center), as Kris receives a National Professorship of Poland in Warsaw, Feb, 2000

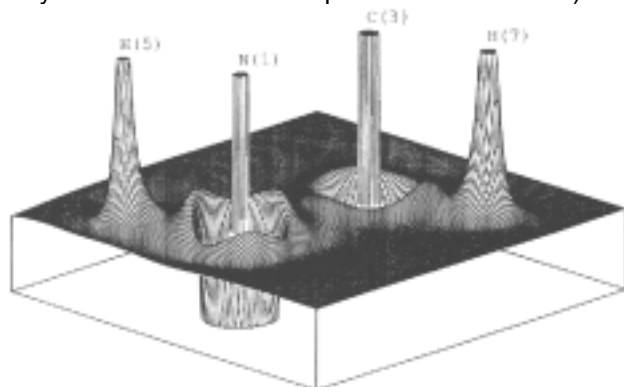
The research of the Matyjaszewski group has been presented at many US and international conferences and has received wide recognition, evidenced by several awards to Kris: Elf Chair of French Academy of Sciences (1998), Humboldt Award for Senior US Scientists (1999), National Professorship of Poland (2000), Fellowship of ACS Polymeric Materials Science and Engineering Division (2001), as well as several visiting professorships and adjunct professorships (e.g. in 2000 at the Polish Academy of Sciences, University of Pittsburgh and University of Pisa).

Miguel Llinás and his group specialize in protein NMR spectroscopy. Combined with X-ray diffraction analysis, NMR is the technique of choice for molecular structure elucidation. However, by contrast with diffraction techniques, the NMR approach can be applied for structural analysis on noncrystalline samples in solution. Thus, NMR facilitates investigation of both structural and functional features, e.g. ligand- or drug-binding, in a rather direct fashion. A major thrust of the Llinás team has been on proteins which have a mosaic structure, with tandem arrays of globular domains of about 5,000-10,000 Dalton each, arranged something like the pearls on a necklace. Many of these proteins are involved in blood clot formation and dissolution, hence understanding their structures and functionality is of utmost biomedical relevance. An interesting feature of these domains is that they also are found in proteins involved in extracellular matrix remodeling, an aspect of relevance

for cell proliferation, embryonic development, cancer and metastasis. Lately, and in parallel with the more biochemical aspects of the research, Llinás has been exploring high-throughput methods for NMR molecular structure elucidation. This involves the development of novel software aimed at expediting the tedious, time consuming process of biomolecular NMR data analysis. The hope is that by bypassing much of the current, labor intensive, NMR analysis, the structure can be reached "directly", via NMR spectroscopic data digitization and "intelligent" automated correlation of data arising from different types of NMR experiments, each of which informs on structural features, but from different perspectives. Such direct procedures, if successful, ought to be applicable, e.g., to fast screening of novel protein motifs arising from current genomic/proteomics research. Besides Miguel, the Llinás group currently consists of a visiting professor, two senior postdoctoral associates, and four graduate students, among which one finds nationals of Argentina, Russia, Sri-Lanka, Switzerland and the USA.

Robert F. Stewart has had a close collaboration with a chemical physics group in the Centre for Crystallographic Studies (CCS) of the Department of Chemistry of the University of Copenhagen since his sabbatical leave there in the spring of 1991. He consults with a group of crystallography students and has been coadvisor to two graduate students—one earned the PhD degree in the fall of 1999, and the other student is expected to complete PhD studies in 2002. The major activity of the CCS is crystallography on proteins, but other areas include (1) the structure and physical chemical properties of chiral molecules, and (2) the determination of electron density distributions and attendant electrostatic properties of molecules and crystals. The latter requires accurate cross-section measurements of x-ray diffraction intensities as well as very high resolution diffraction data (well beyond atomic resolution). Professor Stewart is the principal author of a suite of computer codes known as VALRAY, originally designed to map out the VALence electron densities of molecules in crystals from accurate x-RAY diffraction data. Over the last twenty five years or so it has become clear that the total electron density is the true observable, and that construction of a valence electron density distribution is artificial. The negative Laplacian of the electron density distribution does display the valence structure in the charge density distribution (see an example below). A variety of scalar maps, from the electrostatic potential to the Laplacian of the electron density are determined from x-ray diffraction data with the codes that make up VALRAY. In addition, electric field gradients and the Hessian of the electron density (both second rank tensor properties) in crystals are other examples of electrostatic properties calculated by VALRAY. The CCS has become the home for distribution of VALRAY to other investigators of electron and the total charge density in crystals. Present developments are focused on the determination of the mean thermal electron density as well as properties dependent on the mean thermal charge density. The mean thermal nuclear charge density, usually derived from neutron diffraction data, has

been a feature in VALRAY for the last several years. The CCS was created in 1994 by the Danish Science Foundation. The initial five year funding of 25M Dkr was followed by another five years with 37M Dkr in 1999. The CCS was started by Dr. Sine Larsen, then a lecturer. She is now a full Professor of structural chemistry at the University of Copenhagen and heads up the CCS (on-line information on the CCS may be found at the link <http://www.ccs.ki.ku.dk/>).



The negative Laplacian of the crystal electron density distribution in the mirror plane of the methylammonium cation, showing the valence structure in the charge density distribution.

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ALUMNI NEWS

Your generous responses to the questionnaire in the *Newsletter* and requests for new issues are much appreciated--we now have heard from 280 of you (many more than once as you update us on your whereabouts and careers). Nevertheless, the number of replies was substantially lower this year than in prior years (hope we didn't do a "Florida-count" and lose some replies!) Let's hear from you this year!

S. Donald Hershey, BS 36, who remembers that in 1936, there were four Chemistry majors in the class. He worked for General Electric from 1936 until taking his retirement in 1976. Subsequently, he has relocated from Cleveland to Hendersonville, NC. He writes "It's great to see the way the Department has grown. Congratulations!"

Robert L. Marcus, BS 45, started medical school after his third year at Carnegie Tech. He and his wife continue to work, he as a physician and psychiatrist in private practice, she as Assistant Dean at the School of Social Welfare at the State University of New York at Stony Brook. They have two children. Their son, Davis, is a mathematician working in private industry, and their daughter, Donna, is employed in management and has four children, ages 5 through 11.

Glenn E. Klepac, BS 61, received his Juris Doctorate from the University of Pittsburgh School of Law in 1970 and is currently Intellectual Property Counsel for Alcoa, Inc. since 1979.

Nancy (Wheeler) Tolfa, BS 85, is part owner of NTS Environmental, Inc., an environmental consulting company specializing in "right-to-know" reporting. She is married to Todd Aukerman (CMU BS 85 Chem

E) and they have two children, Andrew, age 3, and Mark, age 1.

Lee Zeiszler, BS 97, is currently attending the Medical College of Virginia at Virginia Commonwealth University and entered the third year medical class in August. He and his wife (Kelley Zeiszler) were expecting the birth of their second child in June (it's a girl!) Their daughter, Karleigh, turned three in June.

GRADUATE STUDENTS

Peter Lycos, PhD 50, reports one way to "go home again"! He writes that when he arrived at Carnegie as an entering grad student fresh out of Northwestern, he began to work with the late Paul Fugassi, who handed him a key to a new lab (i.e., bare lab benches) in a new wing, and told him to report back at the end of the semester with an account of how the students in UG PChem lab had fared. Fortunately, while a senior at NU, Peter had taken a zero credit course in glass blowing, and was able to fabricate the needed equipment. History repeats 50 years later when, as the only Professor of PChem at the Illinois Institute of Technology, he was charged with designing the new PChem undergraduate lab and securing the equipment for the second course in the new two-semester PChem sequence he designed that goes into operation this fall. A new member of the IIT faculty will conduct that lab.

George A. Cowan, DSc 50, informs us that he has made a hobby of retiring and that he has done so many times.

L. Guy Donaruma, PhD 53, is the owner of Pan-Chem Technologies, Consulting Associates. In 1986, he received the CMU Alumni Merit Award for being a nationally recognized scientist. In his spare time, he enjoys golf and bridge.

Marvis E. Hartman, PhD 73, writes that he is back in Pittsburgh after spending four years in Germany with PPG Industries as a Technical Director European Automotive OEM paint business. They miss Europe, but are glad to be back. He is currently directing strategic products/processes for automotive OEM paints at PPG's R & D facility in Allison Park, PA.

Jean M. Donahue, MS 83, has worked as a research associate at Naylor Dana Institute for Disease Prevention, taught at Bernard College and College of Mount St. Vincent, and earned a PhD in Basic Biomedical Sciences from NYU (Jan. 1996). She and her husband, Bart Holland, PhD, will be celebrating their 15th wedding anniversary in June. They have two children, Alicia Marie age 8 and Charlie age 7. She is currently teaching at the Bronx High School of Science, where she advises students doing research projects for the Intel and other competitions.

Robert N. Goldberg, PhD 69, recently moved his office into a newly constructed laboratory at the National Institute of Standards and Technology, where he is actively pursuing research on the thermodynamics of enzyme-catalyzed reactions.

Expanded Departmental Web Site

The next time you visit the department web site you will find that we have a new look to match our ongoing growth. Thanks to our part-time graphic designer, **Nicole Reading**, what you will find includes:

- Research features and upcoming events
- A News and Events section on faculty activities
- Research interest of Chemistry faculty member
- An directory of faculty, staff and grad students
- Educational innovations and outreach programs
- Current and recent issues of the these pages
- Info on the Teaching Lab renovation project

In the works are a redesign of the undergraduate program section of the site and redesigns and expansions of many research group sites. Prior to joining Chemistry, Nicole lived in Chicago and St. Louis where she held positions in print production (including creating color separations for comic books) and web site design. She received a BFA from the School of the Art Institute of Chicago with a concentration in printmaking and computer art.

We welcome your suggestions for further additions or features to the web site. Please feel free to contact Rea Freeland at rf51@andrew.cmu.edu.

Department URL: <http://www.chem.cmu.edu>

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THANKS FOR YOUR SUPPORT!

We want to thank the many Alumni who have made gifts to the University and/or Department. These are extremely important to our efforts to provide a quality educational experience for our students. Tax-deductible gifts may be made directly to the Chemistry Department by explicit request to that effect, or by instructions that your gift to the University be directed to Chemistry. The Department has many activities in both undergraduate and graduate education that benefit from your generosity, including:

- Grants for undergraduate and graduate students for travel to scientific meetings
- Support for Departmental Colloquia
- Support for undergraduate research projects
- The Annual Chemistry Department Retreat

This year we have established an Alumni Fund for student travel to scientific meetings. It is very difficult to get funds to send our students to meetings; almost no money is available in normal grants. This robs our students of participation in national and international meetings--a critical part of their education. Please donate to this fund by mailing your contributions directly to the Chemistry Department. Some of you may be able to take advantage of gift-matching programs at your place of employment. In any case, thanks again for thinking of us!

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2001 ALUMNI QUESTIONNAIRE

Please Complete and Return to
Department of Chemistry
Carnegie Mellon University
Mellon Institute, Box 166
4400 Fifth Avenue
Pittsburgh, PA 15213-2683

NAME:
(Name at CMU if different):

ADDRESS:

PERSONAL HIGHLIGHTS & COMMENTS

BUSINESS TEL:
HOME TEL:
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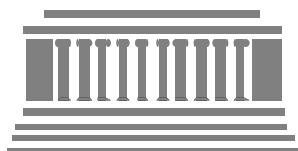
Make address available to Chem Alumni?

Yes

No

CLASS/Degree:
(Please include your degree)

NEWSLETTER
DEPARTMENT OF CHEMISTRY
CARNEGIE MELLON UNIVERSITY



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