The Carnegie Mellon Chemist

CHEMISTRY DEPARTMENT NEWSLETTER

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CARNEGIE MELLON UNIVERSITY

January 2002

No. 12

Chemistry Undergrads

2001 Graduating Class
Twenty-two students received their undergraduate degrees (19 B.S. and 3 B.A.) in chemistry at the May 2001 Commencement. Two students earned Master of Science degrees together with their Bachelor of Science degrees. Two students earned two separate B.S. degrees in both Chemistry and Biological Sciences and two students earned B.S. degrees in Chemistry with an additional major in Psychology. Seven students earned minors in the following areas: two each in Computer Science and Biological Sciences and one each in History, Business Administration, and Engineering Studies. Nine students graduated with University Honors, ten with MCS College Honors, and five students completed the requirements for the B.S. degree in Chemistry with Departmental Honors. One student completed the B.S in Chemistry/Computational Chemistry Track program. Nine students received Carnegie Mellon Senior Leadership Awards, six were inducted into Phi Beta Kappa, three into Phi Kappa Phi and six into Sigma Xi. Three of the graduating seniors were Beckman Scholars and one was an Andrew Carnegie Scholar. One senior was selected to be a Fifth Year Scholar at

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Undergraduate Lab Renovation

Construction is underway for the **MCS Interdisciplinary Undergraduate Science Laboratories**. The laboratories will comprise renovated space in the wing formerly housing the Chemistry Undergraduate Laboratories, plus a newly constructed addition adjacent to that space—see photos on p. 3. The new space, with 100,000 sq. ft. on eight levels (50,000 sq. ft. to be used by Chemistry), will provide undergraduate instruction laboratories for the Departments of Chemistry, Biological Sciences and Physics, and will facilitate a common first-year interdisciplinary laboratory experience for all MCS majors. The analytical and synthetic chemistry labs will occupy one floor each.
The space, designed by Burt Hill Kosar Rittelmann Associates in conjunction with MCS, will include many state-of-the art features in a safe, attractive and flexible environment. The work site now has been topped out—a photo taken earlier in the project shows the juxtaposition of the new and renovated spaces (p. 3). The laboratories will become available on a phased schedule, one floor at a time, with final dedication of the project scheduled for 2003. The laboratories will provide students with facilities to augment experiments with

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Alumna Receives Honorary Degree

Stephanie Louise Kwolek, MM 46, has added another laurel to her burgeoning collection as the recipient of an Honorary Degree from Carnegie Mellon at its 2001 Commencement. The citation read by President Cohon noted that she "spent her 40-year career as a research chemist with the Dupont Company at the Pioneering Research Laboratory in the textile fibers department. Through her work in the field of liquid crystalline polymers, she invented the technology for the foundation of Kevlar fiber, a fiber five times stronger than steel and resistant to wear, corrosion, fatigue and flame. This discovery led to more than 200 applications, including fire-safe suits for fire fighters and bulletproof vests for police officers. A member of the National Academy of Engineering and a recipient of the 1996 National Medal of Technology, she is one of only four women to be inducted into the National Inventors Hall of Fame. For her pioneering discoveries that continue to enhance and enrich our lives, I present Stephanie L. Kwolek for the honorary degree, Doctor of Science and Technology." The twenty or so awards she has received include a Carnegie Mellon University Alumni Association Merit Award in 1983.

The Department Head's Column

It is a pleasure to share our news from 2001 and our future plans with you as the Interim Department Head.

As may be seen elsewhere in this issue, the faculty has seen great success and recognition this year. Our funding continues to be excellent. A recent NSF grant for a new 400 MHz NMR will significantly strengthen our research infrastructure. Kris Matyjaszewski's substantial scientific contributions were recognized by the ACS Award in Polymer Science sponsored by ExxonMobil, the ACS Pittsburgh Award, and induction as a Fellow of the Polymer and Material Science and Engineering Division. Terry Collins was awarded an endowed chair, the Thomas Lord Professorship of Chemistry. Results from Mort Kaplan's collaboration at Brookhaven National Laboratory were described in *Science* and the *New York Times* when they used the RHIC to smash gold nuclei together to create a density of matter that hasn't existed since the Big Bang. Dave Yaron was selected among 127 "New Voices" in *Chemical and Engineering News*. The National Association of Collegiate Scholars recognized Bruce Armitage for his excellence in teaching.

We were joined this year by two outstanding junior faculty, Catalina Achim, an inorganic chemist who rejoins us after a post doctoral position at Harvard, and Danith Ly, a bioorganic chemist who joins us from Scripps Institute (see *Faculty Profiles*). We are delighted with Rick McCullough's appointment as Dean and look forward to his continued leadership in that position. Thanks to many years of dedication by both Rick and Karen Stump, the University broke ground for exciting new Undergraduate Science Laboratories that are now on the way to completion for classes in 2003. Karen Stump's appointment as the new Director of Undergraduate Studies will help us in our ongoing curriculum development. She was awarded a *Responsible Care Award* from the American Chemistry Council in recognition of her teaching excellence. Most recently, we launched a new BS/MS in Chemical Biology, with the support of internships and fellowships from Bristol-Myers Squibb, and we are looking toward more innovations in the coming year. We are conducting searches for a bioorganic chemist and an NMR spectroscopist.

Student and alumni accomplishments are a continuous source of great pride for us. We were pleased that the University awarded an honorary doctoral degree to Stephanie Kwolek, alumna and inventor of Kevlar. The excellent Class of 2001 went to top Ph.D. programs such as at Cal Tech and MIT, and several are pursuing careers at Merck, in medical school, and in the U.S. Navy. Companies like Pfizer and BMS are aggressively recruiting here. Our own recent Ph.D. students are moving on to post-doctoral positions at Cal Tech, Berkeley, Duke, and Scripps. A very generous alumni gift also made possible a Legacy Dissertation Fellowship, awarded to Jeff Pyun in the Matyjaszewski group for research excellence and promise.

The exciting growth and change in the department continues this year and I am pleased to serve as Interim Head and be part of it.

Hyung J. Kim

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Faculty Profiles

This issue profiles two of our new members, both of whom joined the Department as Assistant Professors in the Fall of 2001:

Catalina Achim

obtained her Ph.D. in 1998 from our Department for her study of experimental and theoretical aspects of intramolecular and intermolecular electron transfer involving Fe-S clusters with Dr. Münck and Dr. Bominaar. During her years as a Ph.D. student at CMU, she also investigated diiron-oxo active sites present in new oxygen-activating non-heme enzymes. In 1999 she joined the group of Dr. R.H. Holm at Harvard University as a postdoctoral fellow. She continued to pursue her interest in electron transfer by conducting research on the effect of extrinsic factors on intramolecular electron transfer rates using synthetic mixed-valence complexes. Back at CMU, Catalina will use the experience gained in spectroscopy and in synthetic inorganic chemistry to develop a research program in supramolecular and physical inorganic chemistry. Her research goal is to obtain novel supramolecular structures containing

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Danith Ly

joined the department after postdoctoral stints at UC Berkeley and the Scripps Research Institute. His research covered a wide range of topics, including electron transfer in DNA, natural products, molecular mechanism of human aging, and age-related diseases. His current research interests lie at the interface of chemistry and biology, with emphasis on the development of chemical tools and application of genomics and proteomics technologies to solving problems in biology. Some of the ongoing research projects include regulation of mammalian gene expression, protein engineering, drug discovery, and human embryonic stem cells. With the recent completion of several prokaryotic and eukaryotic genome-sequencing projects, including the Human Genome Project, biological and medical research is presently in the midst of a major transition, driven by the massive sequence information and the development of high throughput (HTP) technologies to exploit its use. However, sequences alone do not tell what all the genes do, how they interact to form a living cell, how the cells assemble to form an

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Chemistry Undergrads

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Carnegie Mellon. Of the graduating seniors, 14 went to graduate school, 7 went to industry and one is attending medical school. Graduate schools to which our majors went include MIT, UCLA, Scripps, UC Davis, Cal Tech, UNC-Chapel Hill, Georgia Tech, UC-Santa Barbara, and Northwestern.

Undergraduate News

- The Department's Student Advisory Council (SAC) has been very active this year under the leadership of David Duran, starting with a departmental picnic at Dave Yaron's home in the fall. Biweekly meetings led to the first departmental Open House over Family Weekend in October. The Undergraduate Chemistry Lounge organized by the SAC brings guest lectures twice monthly on topics of interest to chemistry majors. While most speakers have been chemistry faculty, the group hopes to attract speakers from industry and our alumni.
- Darin M. Flynn has been selected as the 2002 Andrew Carnegie Scholar, a distinction afforded to the top seniors from across the university each year. Darin, who hails from Alaska, has been doing undergraduate research for 2 years in the Collins lab. He plans to go on to medical school at Stanford.
- Four current undergraduates spent a semester abroad during fall 2001. John Ell and Ashish Basuray were down under in Australia at Curtin University and the University of Sydney. Marcy Cook was putting her Spanish fluency to the test at the University of Salamanca in Spain while Christine Siverd was immersing herself in French culture while studying in Avignon, France.
- Lorraine Hsu was selected as a Beckman Fellow following a competitive application and interview process. She joins students from some of the most prestigious colleges and universities in the country (only 20 other schools were selected to participate in this program). Lorraine does research in bioorganic chemistry in the Armitage lab.

Curricular News

The Department has a new degree: a BS in Chemistry/MS in Chemical Biology, to help prepare students for pharmaceutical, biotechnology, and related careers. The program will be open for enrollment in the spring of 2002. In addition to the requirements for the BS in Chemistry, students will take 3 courses in chemical biology, 5 graduate courses, at least one internship, and a thesis project. The program can be completed in 9-10 semesters. Bruce Armitage is the Program Director. Rajesh B. Shukla, PhD89, was instrumental in securing internships and an annual fellowship from Bristol Myers Squib for this program.

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Lab Renovation

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computer simulations, modeling and virtual labs to help promote curriculum growth. Students will be able to practice on a virtual lab, such as that developed by David Yaron, before going on to the real thing. This will promote safe practice with potentially hazardous chemicals, and will help us continue our excellent safety record. Although designed for our undergraduate science instruction, the space will also permit us to expand our pre-K –12 outreach activities. The enhanced space will lesson constraints for on-campus laboratory intensive activities during the academic year, to extend the outreach programs already in place during weekends, and vacation periods of the academic year, and summer months. The estimated project cost is $26.4M, exclusive of new laboratory equipment. As of year-end 2001, $12M of the MCS $15M obligation had been raised. A fund-raising project called "A Landmark Opportunity" has been initiated to help raise the remaining $3M by providing naming opportunities for rooms and laboratory equipment for donors who wish to help push us over the top. To learn more about this, contact Carol A. Cushman, Director of Development; (412) 268-7761 or e-mail: ccushman@andrew.cmu.edu. A link to additional information is provided on the web page of the Department of Chemistry. In addition, we invite you to stop by and see the new labs as soon as they are in use!

An early stage of construction

Artist's rendition of the addition

Outreach Activities

Gary Warnock and his colleagues in the Science Van Outreach Program have had a busy year taking chemistry to K-12 students on behalf of the Department of Chemistry. They performed twenty-five two-hour science shows, over one hundred "hands–on" classroom

sessions, fourteen Saturday workshops for teachers and eight "In-Service" workshops for the Pittsburgh Public Schools. In addition, they participated in various summer programs and have been invited to participate in "science week " activities organized by several area schools. Their program, which encourages undergraduate and graduate involvement, is an asset to the community.
The third year of the Pennsylvania Governor's Institute for Physical Science Education brought 46 teachers from across the state of Pennsylvania to campus from July 8-21, 2001. The fourth session is being planned for July 7-20, 2002.
The Chemistry Department Student Advisory Council participated in the National Chemistry Week celebration at the Carnegie Science Center on Saturday, November 10. The theme this year was *Chemistry and Art*. The students decided to look at the importance of color in chemistry performing various demonstrations such as the Chemical Rainbow and assisted visitors in making slime sculptures.

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Graduate Program

• Ten students completed their Ph.D. over the past year, six students earned Masters Degrees, and one student earned a Master of Science in Polymer Science. This group completed the Ph.D. on average in 5.5 years and has secured prestigious postdoctoral positions at U.C. Berkeley, Cal Tech, Duke, U. of Minnesota, U. of Maryland, and Scripps Research Institute and excellent industrial positions. After restructuring the Ph.D. requirements in 2000, this year the department assessed the changes and found, across the board, that the new requirements have been well received with substantially increased student satisfaction with the research progress report, original proposal, and overall departmental feedback
• **Jeff Pyun** of the Matyjaszewski group was awarded the first Legacy Dissertation Fellowship in September 2001, made possible by a generous alumni gift to the Department. The selection was from among 9 applicants who have reached doctoral candidacy. Jeff's selection as the recipient was based on an impressive record of publications and presentations regarding important contributions in novel inorganic/organic hybrid materials. He expects to defend later this spring and will then take a postdoctoral position where he will work at IBM in collaboration with Jean Frechét and Craig Hawker at U.C. Berkeley. As recipient of this fellowship, he will receive a supplement to his stipend and $500 for travel to conferences. In addition, **Arindam Chowdhury** (Peteanu group) and **Brad Pierce** (Hendrich group) were selected as finalists and will also receive $500 travel awards.• **Nadine Fattaleh** received an Honorable Mention for the 2001 University Graduate Student Teaching Award. She won the Hugh D. Young Graduate Student Teaching Award from the Mellon College of Science in 2000. A quote from one of her former students in organic recitation summarizes quite well the impact Nadine has had on several hundred students throughout her time as a Teaching Assistant, "From other veteran O-chem students, I had learned to dread the course. However, the class ended up being one of my favorites. I can say it was due solely to Nadine." Another student summed up her letter by saying, "Nadine has a true love for teaching and chemistry, which shines through in each class she stands before." Students continue to benefit from Nadine's expertise since for the past 18 months she has held a position as a Special Lecturer in the Department.
• **Missy Pasquinelli** was awarded Honorable Mention for the 2001 Hugh D. Young Graduate Student Teaching Award. As a TA Missy who taught 3 different courses excelled at teaching recitations. One student summarized her strengths, saying, "She was very good at answering questions and throwing them back at the class to see if someone else could come up with the answer. Her questions encouraged understanding of the material, not just 'knowing' it." Missy defended successfully in January, and is off to a postdoctoral position at Duke University.
• **Justin Douglas** and **Brad Pierce** were co-recipients of the Department of Chemistry Graduate Student Teaching Award.

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MCS Dean Appointed

Richard D. McCullough has been named dean of the Mellon College of Science (MCS), effective Aug. 1. In announcing the appointment, President Cohon noted that "Rick brings a great combination of energy, vision and leadership to this position and to the university community, Rick has led the Department of Chemistry through considerable growth including the hiring of five new faculty members, more than $3 million in new instrumentation and infrastructure upgrades, and planning for the $26.4 million undergraduate laboratories in Doherty Hall. He has overseen innovations in the graduate program and recruiting, strongly supported faculty innovation in the undergraduate curriculum and promoted increased concern for diversity."

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Faculty/Staff Affairs

Promotions to ranks with indefinite tenure effective July 2002 for Hyung J. Kim at Professor and Bruce Armitage, Linda A. Peteanu and David Yaron at Associate Professor. Mark Bier received a promotion to Senior Research Scientist.

Josef Dadok and **Aksel Bothner-by**, both emeritus professors of chemistry, have found a new home for the thirty year-old Sigma 5 computer that was an essential component of their then state-of-the-art 250 and 600 MHz NMR spectrometers in the NMR Center for Biomedical Studies. The Computer Museum History Center, located at NASA's Ames Research Center in Mountain View, Calif., decided to add it to their collection since the machine may be the

last of its kind in working order. The computer, which stores 3 MB of data, and has 16 kB of RAM, housed in a file cabinet sized unit, cost $300,000 when new. Sigma computers, which appeared on the market in 1969 and were no longer made after 1975, were widely used in flight simulators, nuclear power plants and in libraries. The machine has proved to be remarkably robust, even surviving an accident in which its circuit boards were drenched with hot water when a nearby pipe ruptured. Joe is helping the personnel of the museum in the transfer of the computer to its new home.

Bothner-by shows the antiquated hard drive of the Sigma 5 computer.
(Darrell Sapp/Post Gazette)

Guy C. Berry will be the guest of honor at a symposium to be hosted by the Mellon College of Science and the Department of Chemistry on 3–4 May in the Mellon Institute Building of Carnegie Mellon. The symposium, which will belatedly mark Berry's 65th year and move to phased-retirement, will provide an opportunity for professional colleagues and former graduate students and postdoctoral associates from the U.S. and abroad to meet and tell Berry what is really going on in polymer science! For details, contact Professor Mohan Srinivasarao (mohan@tfe.gatech.edu).

Ellen Reichenbach, well known to all who graduated in the 80's and 90's, will retire in February following 27 years of service to the Department. As the Undergraduate Student Program Coordinator she has been the Departmental representative who helped students with their scheduling and generally maintained an even keel for all of us with her good judgment and genuine interest in students. Ellen was recognized with an MCS Staff Recognition Award in 1995. In an interview published in these pages several years ago, Ellen was quoted as saying that "One of the best things about this job is getting to know the students individually and one of the saddest is seeing them leave. As a parting thought I would like to encourage all our former students to keep in touch as we all enjoy hearing from you." Her many contributions to the Department and University were celebrated at an Departmental luncheon. Ellen will pass the baton to **Patsey Haddock**, who will move from her position as Financial Assistant in the Department. More on Patsey in a future issue.

Karen H. Stump has been appointed Director of Undergraduate Studies, replacing **Charles H. Van Dyke**, who served in that position with distinction for many years. Chuck will continue to serve as freshman advisor and to work with prospective freshman in our recruiting efforts. Karen will continue as Director of Laboratories and as the department representative to MCS' Committee on Undergraduate Affairs and to the Undergraduate Laboratory Renovations. In these roles, Karen will play an expanded role in curriculum discussions and as the key point of contact for internal and external questions about the undergraduate program.

Kris Matyjaszewski and **Guy C. Berry** have established a new Editorial Office at Carnegie Mellon for the journal *Progress in Polymer Science*; they are co-editors for the journal. *Progress*, which enjoys a high citation rating in its field, provides critical reviews in its subject area.

Mort Kaplan has received a courtesy appointment in the Physics Department of Carnegie Mellon.

Hyung J. Kim has been Interim Head of Chemistry since November, 2001. A Research Profile on Kim may be found on p. 7.

Mark Bier and **Neil Donahue** are currently officers in the Pittsburgh Section of the American Chemical Society. Mark is the Chair and Neil is the Secretary–Elect. G. C. Berry continues as a Section Director.

Evelyn Scannell

will be remembered by the "more mature" alums and faculty of the Department as the secretary to the Chair of the Department of Chemistry when she retired in 1976, after seventeen years of service to Carnegie Mellon. We regretfully report that she passed away on Dec., 26, 2001 at age 95. She remained active in community affairs, receiving the Jewish Community Center Achievement Citation for Senior Adult Volunteer Work on her 90th birthday in 1996.

A Nobel Connection

John F. Nash Jr., the Nobel Laureate who is the subject of a recent movie, has a Carnegie Mellon connection not mentioned in the movie. He enrolled in (then) CIT in 1945 on a George Westinghouse Scholarship to study chemical engineering, switching after one year to chemistry (he disliked his mechanical drawing required course), and then to mathematics after he encountered quantitative analysis. In the end, he was granted an M.S. and a B.S. in mathematics—then on to Princeton University, and the work that would eventually bring him the Nobel Prize.

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Faculty Awards

Bruce Armitage received the *2001 Nontenured Faculty Award*, sponsored by the 3M Corporation, and was recognized for excellence in teaching by the National Association of Collegiate Scholars.

Karen Stump has received the regional *Responsible Care Catalyst Award* for college and

university teachers from the American Chemistry Council. The award is based on teaching excellence in the classroom and academic laboratory, committee activities, civic involvement, and other similar contributions which enrich teaching.

Terrence J. Collins has been named the *Thomas Lord Professor of Chemistry*. A champion in the field of green chemistry, Collins has gained international recognition for his work in creating a new class of oxidation catalysts with the potential for enormous, positive impact on the environment. He is the director of Carnegie Mellon's Institute for Green Oxidation Chemistry. Prior honors include the Environmental Protection Agency's 1999 Presidential Green Chemistry Challenge Award and Japan's Society of Pure and Applied Coordination Chemistry Award. Collins is an honorary professor of the University of Auckland, New Zealand, a fellow of the Alfred P. Sloan Foundation and the World Innovation Institute, and a Dreyfus Teacher-Scholar.

Krzysztof Matyjaszewski, J. C. Warner Professor of Natural Sciences, received the ACS Pittsburgh Section's *Pittsburgh Award* in October 2001, and will receive the *2002 ACS Award in Polymer Science* during the National ACS Meeting in Orlando, FL, on April 7, 2002. The *Pittsburgh Award* cites Kris' creative, significant and extensive research, publishing and journal editing, his teaching and student mentoring, his university leadership positions and his multi-faceted interactions with local chemical companies. Past chemistry faculty who have received the Pittsburgh Prize include John C. Warner (45), Frederick D. Rossini (59), John A. Pople (75), Robert B. Carlin (81), Aksel A. Bothner-By (88) and Guy C. Berry (94). The *ACS Award in Polymer Science* cites "his research accomplishments in advancing the science and technology of polymerization methods. " Those methods have focused on methods to carry out radical polymerizations to prepare polymers with well-defined composition, structure and molecular weight. The industrial interest in the process is demonstrated by a consortium of 21 industrial companies from around the world interested in creating novel polymeric materials that Kris directs at Carnegie Mellon.

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Faculty Profiles *(Continued from p. 2)*

Catalina Achim
multiple transition metal ions. These structures offer the opportunity to employ the rich aspects of electronic structure and physico-chemical properties normally displayed by transition metal ions to achieve novel electric, magnetic, and chemical properties for the supramolecular systems. The assembly of one-, two-and three-dimensional structures containing metal ions bridged by polydentate ligands will be based on principles of coordination chemistry and of molecular self-assembly and recognition manifested in biological systems. Catalina will explore the possibility of using DNA-like structures as scaffold for organization of metal ions in linear arrays that may function for example as conduit for electron transfer. These molecules have potential applications in nanotechnology, molecular electronics, and molecular recognition.

Danith Ly
organism, or what goes wrong in a disease. Researchers are facing a daunting task in trying to understand the dynamics of gene expression and the function associated with each expression cascade. The goal of the post-genomic era is not simply to provide a catalogue of all the genes, but rather to understand how they function together in the context of an intact living cell and organism. By integrating chemistry with cellular and molecular biology, he hopes to develop chemical tools to regulate gene expression, and hence, elucidating the mechanism of physiological processes of critical importance relating to development, aging, and aged-related diseases.

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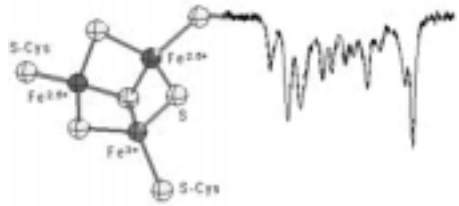
Research Profiles

Eckard Münck and his group specialize in Mössbauer spectroscopy and Electron Paramagnetic Resonance, focusing on the active sites of iron-containing metalloproteins. Many proteins and enzymes contain unique metal clusters that catalyze spectacular chemical reactions. For instance, the cofactor center of the enzyme nitrogenase, a cluster comprising seven iron atoms, one molybdenum atom and nine sulfido groups, performs a 6-electron reduction of dinitrogen to yield ammonia. Another example involves the enzyme sulfite reductase which catalyzes the 6-electron reduction of sulfite to sulfide, utilizing an assembly consisting of a porphyrin covalently linked to a cuboidal [4Fe-4S] cluster; this novel active site assembly was discovered by the Münck group via a detailed Mössbauer study. The logo of the Münck lab shows a so-called 3Fe-4S



cluster attached to a Mössbauer spectrum. The Münck group discovered this cluster in 1979 in an electron transfer protein; subsequent research in many laboratories has shown it to be a fundamental structure ubiquitously distributed in nature. The four sulfides bridging the iron atoms provide a pathway for antiferromagnetic interactions; this is not unusual as it has been observed for a variety of cluster types found in biological systems. What was unusual was the observation, made by Mössbauer spectroscopy, that the electron transferred to the cluster delocalizes over two iron atoms, giving rise to a valence-delocalized pair. The 'traveling' electron promotes parallel alignment of the unpaired spins of the two iron sites by a mechanism termed double-exchange. Analysis of the Mössbauer spectrum in the logo placed the concept of double exchange into the chemical literature. Many groups are currently inter-

ested in double exchange as this interaction can be exploited for the design of molecular magnets and, moreover, consideration of double exchange has given new insights into the mechanism of electron transfer in metalloproteins. Emile Bominaar, a very productive theoretician on our research faculty, has led the way in providing a theoretical underpinning to double-exchange linked electron transfer. The Münck group also studies higher oxidation states of iron complexes as they occur during the catalytic cycles of enzymes. The group described a novel diiron(IV) cluster in the catalytic cycle of methane monooxygenase, the enzyme that converts methane into methanol. The Münck group has collaborations with over 20 research groups in the U. S. and Europe; the coworkers include chemists, biochemists, physicists, geneticists and microbiologists. Collaboration with colleagues at the University of Minnesota, recently reported the first diiron(IV) synthetic complex that can serve as a structural model of the methane monooxygenase intermediate; the complex is also a spectacular catalyst.

Hyung Kim and his group work on theoretical chemistry applied to condensed-phase chemical reactions and dynamics. It is well-known that in solution, the solvent environment can significantly alter the mechanisms and controlling factors of chemical reactions, e.g., electron/proton transfers and S_N1/S_N2 reactions. Similarly, relaxation dynamics and related spectroscopy, e.g., dielectric relaxation and far-IR spectroscopy, may be significantly modulated by a solvent environment, compared to the gas-phase. However, little is understood as to the details of these solvation effects at the molecular level. To gain insight into this, Kim and his students develop theoretical models and implement them with modern computational chemistry techniques. One of their recent accomplishments is the construction of a computationally-efficient quantum-mechanical solvent electronic description via a truncated adiabatic basis-set (TAB) representation. This properly captures both the linear and nonlinear molecular polarizabilities and allows electronic excitations for the solvent molecules. Its implementation via molecular dynamics (MD) computer simulation algorithms and application to water and aqueous solutions have provided new insight into many long-standing issues associated with various spectroscopies of water. For example, their MD study showed that the 800cm^{-1} structure of depolarized Raman spectra under ambient conditions arises from the nonlinear electronic response of water to its librational motions. They were the first to calculate the condensed-phase photoabsorption band of liquid water, and clarify the origins of its blue-shift and red-tail. The current thrust is to extend the TAB description to study dynamics and spectroscopy under different thermodynamic conditions, such as water clusters and ice. Solution-phase quantum chemistry employing Onsager's reaction field approach is another active research area of the Kim group. Their recent focus is developing a reaction field theory to study equilibrium and nonequilibrium solvation in quadrupolar solvents, such as benzene and supercritical carbon dioxide. In addition, they have several ongoing collaborations on Brownian dynamics simulations of macromolecules and chemical reactions in highly-concentrated ionic systems with researchers in Korea and Russia, as well as in the US. Last year Kim visited Seoul National University in Korea as a Distinguished Visiting Associate Professor of the Brain Korea 21 Project in Spring and the University of Colorado, Boulder as Visiting Associate Professor in Fall.

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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 nearly 300 of you. As usual, capsules from your questionnaire responses are included below, but in this issue these are augmented by tidbits we picked up over the year. Some of these came via phone calls by Rick McCullough, Karen Stump, Chuck Van Dyke and Patsey Haddock as part of Dean McCullough's initiatives to keep in touch with alumni.

Robert N. Anderson, BS42, writes, "Sure enjoy these letters. Some of these research projects are really interesting and I must admit are over my head. Thanks for these letters."

Thomas J. Byrnes, BS58, lives in Annandale, Virginia. In September 2001, he retired from the Department of Justice after 39 years as a patent attorney. At the time of his retirement, he was an assistant director in the Commercial Litigation Branch and Senior Level Patent Counsel for the Civil Division. He and his wife of 45 years, Camille C. Porter (MM51), plan to travel and spend more time with their seven grandchildren.

Kenneth E. Daugherty, BS60, has retired as a Regents Professor of Chemistry from the University of North Texas, in addition to retiring as a Bird Colonel in the Army Chemical Corps Reserves. He was also a professor at the University of Pittsburgh. He has been cited in Who's Who in the World; Who's Who in America, and Who's Who in Science and Engineering. He is President and CEO of The KEDS, Inc.

Joseph P. Yevich, BS62, PhD69, has worked for 31 years with Bristol-Myers Squibb Company. He is currently Director of Core Chemistry at the company's Wallingford, CT research facility. He and his wife Mary have two grown children, Paul and Eileen and a two-year old granddaughter, Brianna. Dr. Yevich enjoys golf and tennis. He maintains being a die-hard Pirates and Steelers fan.

Steven G. Link, BS72, completed 23 years with Eastman Kodak Company in April of 2000. He was also appointed Laboratory Head of the Dye Research Laboratory of the Imaging Materials Division, Kodak Research and Development.

Peter J. Spohn, BA73, is now an orthopedic trauma surgeon in private practice in South Carolina. He, his wife Verna, and daughter Carole Ann are very happy in the Coastal South. Dr. Spohn writes that he is "quite impressed with how the department and the University have kept up with the times."

Joseph Weiss, BS78, received his MBA from Case Western Reserve University in 1984. Dr. Weiss is currently employed by Rhodia. He and his wife, Donna, have two children, Alyson (11) and David (7).

Leanne J. Henry, BS82, is transferring to the Pentagon from West Point, where she was an instructor in the Physics Department. She will be at headquarters USAF on the Air Staff and will be involved in science and technology planning for the Air Force.

Nils Adey, BS83, worked as a Research Associate from 1983–1985 at Garex Labs and Meloy Labs in the Washington, D.C. area. He received his Ph.D. in Microbiology in 1991 from the University of North Carolina, Chapel Hill in the laboratory of Dr. Clyde Hutchisons. His postdoctoral fellowship was served from 1992–1995 at the University of North Carolina, Chapel Hill in Dr. Brian Kay's lab. Since then, he has been a scientist at Myriad Genetics (1995–2000) in Salt Lake City, Utah and is currently Director of Molecular Biology at Biomicro Systems which is also located in Salt Lake City, Utah.

Andrew A. Sicree, BS83, MS85, became a proud father again on June 4, 2001, when his wife Rebecca Marie Sicree (MS87 Electrical Engineering) gave birth to their sixth child, Genevieve Marie. Mother and child are doing well, and little Genevieve was welcomed home by five brothers and sisters: Alexander Joseph (9), Thomas Ignatius (7), Teresa Rose (4), Maria Kateri (3) and Isabel Ann (1). Genevieve is named for St. Genevieve, the patroness saint of Paris and for Our Lady. Dr. Sicree is the director of the Earth & Mineral Sciences Museum and a member of the faculty at Pennsylvania State University.

Sheila (Bomberger) Ricks, BS89, is a technical sales representative for Lincoln Electric. She has a son, Daniel, who is one year old. She loves to hear from old classmates.

Joanna Downer, BS93, who received her PhD in nuclear chemistry from Washington University in 1998, returned to campus to speak to the undergraduate seminar and to Women in Science, on October 25. Joanna talked with the students about her chosen career as a science writer. She is currently at the Johns Hopkins Medical Institutions covering their stem cell and genetics/genome centers.

John Nadzum, BS93, has been with McNeil Consumer Healthcare since 1995 in their R&D Support to Marketed Products group. John spent a lot of time at their plant in Round Rock Texas and contractors in KY, OK, NJ, and NY. He has been doing a lot with product transfers, scale-up, trouble shooting, and equipment evaluation. He spent the first 4 months of 2000 in China as the lead R& D person for the construction/expansion of McNeil's new plant in Shanghai. He is currently on a 3-year assignment as the on-site R& D person for their largest plant, in Las Piedras Puerto Rico. Also, as a hobby, John and some friends run a Japanese animation festival.

Amy Pfizenmayer, BS93, now Ratnaparkhi, finished her PhD in organic chemistry at the University of Pennsylvania and then went to work at Berlex Laboratories in the Medical Writing field. During the summer she found herself moving back to Pittsburgh with her husband and one year old daughter.

Matthew J. Solitro, BA97, graduated from the University of Pittsburgh School of Medicine with his MD this May. In July, he began his 3 year residency in Internal Medicine at Brown University's Rhode Island Hospital.

Lee Zeisler, BS97, stopped by the office in mid January while making the rounds to some area medical schools and hospitals. Lee is receiving his M.D. this year and will be pursuing a residency in radiology. His third daughter is due any time.

Johanna Bechtel, BS98, is working for Accenture Technology Labs in Palo Alto, California where she says, "I'm still doing labwork, but it's computer/technology innovation labs instead of the chemistry kind--who knew how helpful learning java coding was going to be for me!"

Elizabeth Kanabe, BS98, is utilizing her Masters degree from the Heinz School in the area of Health Care Policy and Management having just accepted a new position in hospital planning and administration. Elizabeth was a swimmer while a student and has been keeping healthy by training for and running marathons.

Makenzie Newman, BS00, is working on drug therapies for hepatitis C at DuPont Pharma in Delaware, which has been acquired by Bristol-Myers Squibb.

Izzat Raheem, BS00, with Computational Chemistry track '00, is currently working for Merck. He is returning to campus January 31 to hold an information session about opportunities at Merck. He will be interviewing students for full time positions and internships while he is here.

Eric Silverman, BS00, is in his second year of graduate school at the University of Florida. His thesis project deals with transition metal complexes.

Tejal Teli, BA00, had been teaching mathematics in a private school in the Philadelphia area. She has recently relocated to New Jersey to be closer to her family. She is planning on attending graduate school for a Masters in Social Work.

Narin Wongngamnit, BS01, is currently a first year medical student at the Indiana University.

Graduate Students

Elizabeth (Pearsall) Hartner, MS37, says this year she is helping with platinum (!) reunion plans. She volunteers at the Carnegie Museum of Natural History and writes reviews for science books and films.

Alan B. Rothman, MS52, PhD54, has been employed part-time as a staff temporary appointee with the Transportation of Hazardous Materials Section of the Energy Technology Division since 1992; he retired from full-time employment at Argonne National Laboratory. His R&D efforts have involved: generation and combustion of hydrogen in storage and transportation of detinide materials; development of a process system for conversion of depleted uranium hexafluoride stockpile, from past uranium enrichment

operations, to more manageable and useful products; and methods to disperse and degrade oil spill crude oil at sea to mitigate shoreline contamination. He is enjoying snow skiing and dancing in his semi-retirement, and reports he enjoys reading about innovative research at CMU.

John R. Peffer, PhD58, retired after 30 years with Coatings Research at PPG Industries. Now he enjoys golf and bridge. He also volunteers in the community and in his church.

John J. Krajewski, PhD59, is retired as the Manager of New Ventures Polymers at Allied Signal Corporation since 1996.

Frank J. Millero, MS64, PhD65, received the first ACS Geochemistry medal at the 221st ACS National Meeting in San Diego in April, 2001. He recently published another book, "Physical Chemistry of Natural Waters", Wiley, 2001. After working as a physical chemist with Esso Research & Engineering Co., he joined the University of Miami in 1966.

Shean-Jer (Sam) Chen, PhD89, writes "It is nice to receive the newsletter. I am a little disappointed to know Dr. Berry is retiring."

Rajesh Shukla, PhD89, is currently employed by Bristol-Myers Squibb. Rajesh worked with members of the department to institute a Bristol-Myers Squibb fellowship for the new BS/MS in Chemical Biology.

Kim Kostka, PhD93, is very busy with her 2 year old daughter and teaching general chemistry and laboratories and organic laboratories in Wisconsin.

Rob Loewe, PhD00, is currently a postdoctoral fellow with Jon Lindsay at North Carolina State. He is currently starting his job search.

Kelly Davis, PhD01, is very happy as a postdoctoral fellow in Colorado. She is currently working on a variety of projects including degradable polymers for tissue engineering purposes, DNA delivery systems and cellular degradation.

The Departmental Web Site

Regular improvements and additions to the department web site continue. A new undergraduate web site, which went live last spring, includes descriptions of degrees and options, courses descriptions, undergraduate research opportunities, and information for prospective majors. Chemistry faculty with new or expanded sites include: Bruce Armitage, Terry Collins, Rea Freeland, Hyung Kim, Tomasz Kowalewski, Danith Ly, and Dave Yaron. Expanded graduate student section, more expansions of the research group sites and photos of the new labs are in the works. As always,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. Please visit us at **http://www.chem.cmu.edu**

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PERSONAL HIGHLIGHTS & COMMENTS

NEWSLETTER

DEPARTMENT OF CHEMISTRY

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