

# The Carnegie Mellon Chemist

## CHEMISTRY DEPARTMENT NEWSLETTER



CARNEGIE MELLON UNIVERSITY

February 2003

No. 13

### Chemistry Undergrads

#### 2002 Graduating Class

Nineteen students received their B.S. degrees in chemistry at the May 2002 Commencement. Members of the graduating class demonstrated a wide range of interests beyond chemistry. In addition to their BS in chemistry, two students earned Master of Science degrees together with their Bachelor of Science degrees, one each had majors in Spanish and French, and one student earned a B.F.A. in music. A student earning a B.S. in Materials and Engineering Science, had a major in Chemistry. Five students earned minors in the following areas: two each Biological Sciences and one each in Engineering Studies, Ethics and Computer Science, and Psychology. One student in each of the Department Options for Polymer Science, Management and Computational Chemistry. Many members of the 2002 Graduating Class received honors in recognition of their scholarship: nine students graduated with University Honors, seven with MCS College Research Honors, and two students completed the requirements for the B.S. degree in Chemistry with Departmental Honors. Six students received Carnegie Mellon Senior Leadership Awards, five were inducted into Phi Beta

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### Celebrating the Interdisciplinary Undergraduate Science Laboratories

A new age has dawned for laboratory-based instruction of Carnegie Mellon undergrads: the new Undergraduate Science Laboratory wing is in operation. The University community got an early look at the new labs during the October 4 Homecoming. Following a ceremony in the new 125-seat MCS Lecture Hall, the Carnegie Mellon community participated in an open house with



*Exterior view of the new lab wing*

hands-on activities and toured the exciting eight-story facility, designed to serve the lab-based teaching needs of the Departments of Chemistry, Physics and Biological Sciences. Speakers included Jared

Cohon, Rick McCullough, Karen Stump, and Barry Luokkala. Photos of some of the interesting architectural and technical features may be found at the url:

([www.cmu.edu/mcs/uglabs/index.html](http://www.cmu.edu/mcs/uglabs/index.html)).

For example, the unique glass-enclosed exterior chase for the ventilation ductwork blends Carnegie Mellon's classic Hornbostle design with 21st century needs.

In addition to labs for Chemistry and Physics, the new facility provides a large space for a freshman Interdisciplinary Laboratory, to provide students with an integrated lab experience in chemistry, physics and biology. The labs' innovative features accommodate the latest scientific equipment and computing resources for undergraduate instruction. The addition incorporates a conference room, computer cluster, study room, staff offices, chemical storage space, and an outreach lab.

The design of the three chemistry laboratories (analytical, physical and synthetic) maintains an open environment with good line-of sight for safety purposes, and wide aisles to facilitate the movement of students and mobile instrumentation. High levels of natural and artificial light, along with a sound system and the

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## The Department Head's Column

It is a pleasure to update you on the exciting events in the Department of Chemistry this year.

I am pleased to report the department's outstanding research accomplishments, including some exciting distinctions. Our research in organic and polymer chemistry is ranked second in the U.S. by InCites for average citations per paper. Also, Guy Berry was appointed University Professor, Carnegie Mellon's highest rank, and was also selected as a Fellow of the ACS Polymeric Materials: Science and Engineering (PMSE) Division. He was also honored with a special 65<sup>th</sup> birthday symposium highlighting his tremendous impact on physical polymer chemistry. Kris Matyjaszewski earned the 2002 ACS Award in Polymer Science for extensive and creative accomplishments in polymer science. Terry Collins earned an endowed chair, the Thomas Lord Professor of Chemistry, honoring his leading work in green chemistry. Traian Sarbu, a postdoctoral associate in the Matyjaszewski group, shared in this year's Presidential Green Chemistry Challenge Award, an award received by the Collins' group in 1998. Dean Rick McCullough received the ACS Akron Award for chemists under 45 years old. Mort Kaplan became Deputy Council Chairperson of the 45-university STAR Collaboration. Aksel Bothner-By received the Gunther Laukien prize for NMR research. Finally, our sponsored research budget has increased by 39%.

We are equally delighted with our educational accomplishments. The new Undergraduate Interdisciplinary Science Laboratories are now open, providing 100,000 square feet of state-of-the-art space for chemistry, physics and an innovative interdisciplinary freshman lab. The sophomore analytical lab and the junior physical chemistry labs will be held in these beautiful facilities this spring. Of course, none of this would be possible if not for the tireless dedication and exceptional skills of Karen Stump. For her outstanding work as an educator and leadership in laboratory education, Karen was also awarded the regional Responsible Care Catalyst Award from the American Chemistry Council. David Yaron received the Julius Ashkin Award for excellence in teaching in the Mellon College of Science.

The past year has also brought growth in the area of NMR, a long-time strength of our department. Roberto Gil joined us as NMR Spectroscopist and Research Scientist and has been leading our efforts to set up new 500 MHz and 300 MHz instruments in soon-to-be completed space. We are in the process of searching for two new faculty, one in materials and another in theoretical/computational chemistry, who will help us build further bridges across disciplines.

Finally, we awarded 17 B.S. and two B.S./M.S. Honors degrees to 2 of our consistently high caliber of undergraduates and 13 Ph.D.'s to our outstanding graduate students. Their diverse talents are taking them to UC Berkeley, Cal Tech, Georgia Tech, Duke, Merck and PPG as well as Stanford Law and the Peace Corps. It is rewarding to serve as department head to facilitate the accomplishments of the great talent here among the students and faculty.

Hyung J. Kim

### Chemistry Faculty:

C. Achim  
B. A. Armitage  
G. C. Berry  
T. J. Collins  
N. Donahue\*  
A. J. Gellman†  
S. T. Graul  
R. Freeland  
M. P. Hendrich  
M. Kaplan

P. J. Karol  
H. J. Kim  
T. Kowalewski  
M. Llinás  
D. Ly  
K. Matyjaszewski  
R. D. McCullough  
E. Münck  
G. D. Patterson  
L. A. Peteanu  
S. W. Staley

R. F. Stewart  
K. H. Stump  
C. H. VanDyke  
L. M. Walkert  
G. Warnock  
D. Yaron

### Research Scientist

M. E. Bier  
E. Bominaar  
C. Horwitz

### Resident Emeriti

A. A. Bothner-By  
E. F. Casassa  
A. A. Caretto Jr.  
J. Dadok  
R. L. Kay  
T. P. Kohman

\*Joint with ChemE  
†Courtesy, in ChemE

## Faculty Profiles

This issue profiles two members of the Chemistry faculty:

### Karen H. Stump

joined the Department of Chemistry in 1983, following three years at Washington and Jefferson College (1980-83). She is now Principal Lecturer and the Director of Undergraduate Studies in Chemistry. An alumna (M.S. 1981), Karen is certainly well-known to the many Carnegie Mellon alumni who have taken or worked as teaching assistant in laboratory courses in the Chemistry curriculum since she joined our faculty. In addition to her teaching responsibilities in Laboratory I: Introduction to Chemical Analysis, and her duties as the Director of Undergraduate Studies, she has devoted an alarmingly large effort to the development of the new undergraduate teaching laboratories, highlighted elsewhere in this issue. From planning to construction, the project has spanned four Department Heads (Berry, Matyjaszewski, McCullough and Kim), two Deans of the Mellon College of Science (Henry and McCullough), two Provosts (Christiano and Kamlet) and two

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### Garry F. P. Warnock

joined Carnegie Mellon as a Visiting Professor in August of 1997, becoming a Senior Lecturer and the Director of the Van Outreach Program in the Chemistry Department in the Fall of 2002. After receiving his Ph.D. degree in Inorganic Chemistry from the University of Minnesota in 1985, Warnock spent 3 years as a post-doctoral fellow with Dr. Martin Bennett at the Australian National University. He was a visiting professor at the University of Pittsburgh before joining Carnegie Mellon, teaching and working with Professor Henry Bent to develop a science van outreach program at Pitt. He was appointed to teach courses in the undergraduate curriculum and to design and establish an Outreach program to the schools in the Pittsburgh area. A principal feature of the Outreach activity, The Carnegie Mellon Science Van Outreach Program, came into being in early 1998 with the generous support of the Eden Hall Foundation. Since that time it has successfully continued to solicit contributions from other local foundations and societies, including the Laurel Foundation, the Howard Hughes Medical Institute, the Spectroscopic

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## Chemistry Undergrads

*Continued from page 1*

Kappa, five into the National Society of Collegiate Scholars, three into Phi Kappa Phi and three into Sigma Xi, two into Mortar Board, and one each into the Phi Sigma Iota and Lambda Sigma Honor Societies. One student was an Andrew Carnegie Scholar (funded by Carnegie Mellon's alumni through the Andrew Carnegie Society), and one student attended Carnegie Mellon on a Presidential Scholarship. One senior was awarded a Merck Summer Fellowship in Computational Science after his first year. Of the graduating seniors, five plan to enter graduate school, five plan to enter a medical school, five plan to enter industry and two plan to study law. Graduate schools to which our majors went include UC-Berkeley, George Washington University, UNC-Chapel Hill, Georgia Tech, and the Heinz School of Carnegie Mellon.

### Undergraduate News

• The Department's Student Advisory Committee (SAC) has remained active this year, with continuing activities to develop relationships between faculty and students. A departmental picnic was again held at Dave Yaron's home this fall, as was a Halloween dinner at Karen Stump's. This spring Stu Staley and his wife will again host a breakfast for students, and Paul Karol has agreed to host a function as well. The SAC has also continued to participate in outreach activities by setting up a table at the science center during the ACS National Chemistry Weekend. Over the course of the weekend approximately 3,000 young students from the area attend the show and get to learn more about Chemistry in the process.

• Darin M. Flynn was 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 will be off to medical school at Stanford this fall.

- Mike McEwan participated in the Students Abroad program, with studies at the University of London in the fall 2002.
- Dante Romanini became the first student to enter the Department's new degree program leading to a BS in Chemistry/MS in Chemical Biology, to help prepare students for pharmaceutical, biotechnology, and related careers. Rajesh B. Shukla, PhD89, was instrumental in securing internships and an annual fellowship from Bristol Myers Squibb; Dante was the recipient of an internship at BMS last summer. Professor Bruce Armitage is the Program Director.
- Daniel Vogel, a graduating senior this year, was awarded a Merck Summer Fellowship in Computational Science after his first year. The Fellowship was created via a grant from the Merck Company Foundation to the Mellon College of Science to create a new program and stimulate interdisciplinary research in Computational Biology and Chemistry. The summer fellowships are awarded via a competitive application process to encourage talented students to work on problems of potential interest in computational chemistry and biology. Dan first worked with Professor David Yaron of this department on Parallel Processing Issues in Computational Chemistry, and as a software developer at TSI/Gross Profit the following summer.

### Curricular News

The Department has added new required courses in adding Math Methods for Chemistry and Modern Analytical Instrumentation to better prepare our undergraduates for their future in graduate schools or industrial laboratories, etc.

### New Undergrad Labs

*Continued from page 1*

latest in computer-controlled ventilation, all contribute to a great new working environment. Students will enjoy expanded opportunities for interdisciplinary exploration and team projects. The new curriculum already developed for this space will involve freshmen in activities on forensic science.



*Lower-level entrance to the Labs*

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 during enhanced weekends, and vacation periods of the academic year, and summer months.



*Analytical chemistry lab*

The Chemistry Department extends thanks to the more than 200 alumni who made gifts in support of these laboratories, particularly leadership gifts (\$1000 or more) from chemistry faculty and alumni: Guy C. Berry, Margaret Carver (S 1943), Rick McCullough, John V. Nelson (S 1976), and Karen Stump (S 1981). 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 Sharon L. McCarl, Associate Dean, MCS; (412) 268-3018 or e-mail: sm5r@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 if have the opportunity!

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## Graduate Program

Our recruiting efforts were especially successful for 2002-2003 with nineteen students currently in the first-year of the program. Many thanks go to Eckard Münck for outstanding work in this area. We also graduated twelve Ph.D. students during 2002, who went on to postdoctoral positions at UC Berkeley, Scripps, U. Minnesota, Duke, and Cal Tech.

A number of our students were honored for academic excellence. Ben Janesko and Audria Stubna each received NSF Graduate Research Fellowships, providing them with five years of stipend support.

Tomislav Pintauer and Bhaskar Datta shared the Harrison Legacy Dissertation Fellowship, established by John Harrison (S 1962).

**The Bayer Foundation** has awarded a \$583,000 grant to the Chemistry and Chemical Engineering departments for innovative graduate fellowships. The Bayer Fellows, co-advised by a chemist and a chemical engineer, will gain experience in interdisciplinary collaboration. They will also participate in summer internships where they can learn in greater detail the expectations of industrial research.

These funds will be used beginning in 2003 to support two Ph.D. students doing interdisciplinary research in chemical engineering and chemistry, particularly in the areas of polymer characterization and computational chemistry and modeling, and one Ph.D. student doing

research in process systems engineering.

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## Faculty/Staff Affairs

**Hyung J. Kim** has been named Head of the Department of Chemistry—he had been the Interim Head of Chemistry since November, 2001. A Research Profile on Kim was included in a preceding issue of this Newsletter.

**Richard D. McCullough**, Dean of MCS, received the ACS Akron Award chemists under 45 years old working in any branch of chemistry and living within 300 miles of Akron who "demonstrate exceptional promise for making significant contributions to chemical science."

**David Yaron** received the Julius Ashkin Award for excellence in teaching in the Mellon College of Science.

**Aksel A. Bothner-By** was recognized for his accomplishments in NMR research by two awards: an award from the Eastern Analytical Symposium in November, and the Günther Laukien prize of the Experimental NMR Conference in April.

**Guy C. Berry** was appointed University Professor, which is Carnegie Mellon's highest rank. He was also selected as a PMSE Fellow of the American Chemical Society Division of Polymeric Materials: Science and Engineering for significant accomplishments in physical polymer chemistry. Previous University Professors in the Chemistry Department have been Aksel A. Bothner-by and John A. Pople.

**Krzysztof Matyjaszewski**, the *J. C. Warner Professor of Natural Sciences*, received the *ACS Award in Polymer Science* from the Polymer Division of the American Chemical Society in March, for his research accomplishments in advancing the science and technology of polymerization methods. He also received an honorary degree (Doctorate Honoris Causa) from the University of Ghent, Belgium, in April 2002.



*Matyjaszewski accepting the Polymer Science Award of the Am. Chem. Soc. from Elsa Reichmanis, ACS President.*

**Traian Sarbu**, Post-doctoral Fellow, shares a Presidential Green Chemistry Challenge Award with Eric Beckman group at the University of Pittsburgh.

**Mort Kaplan** became Deputy Council Chairperson of the 45-institution STAR Collaboration operating the STAR experiment at the Relativistic Heavy Ion Collider at Brookhaven National Laboratory.

**Rea Freeland**, Associate Head of Chemistry, has been named the Associate Dean of Special Projects in the Mellon College of Science. She will share her time between these two assignments.

**Karen Stump** received the regional *Responsible Care Catalyst Award* from the American Chemistry Council honoring teaching excellence among college and university teachers.



*Provost Kamlet presents the Responsible Care Catalyst Award to Karen Stump*

**Terrence J. Collins**, has been named the *Thomas Lord Professor of Chemistry*, in recognition of his research in green  
*Continued next page*

## Berry Symposium

**Guy C. Berry** was treated to a two-day Symposium at the Mellon Institute in May to recognize his contributions to polymer science. The event, organized by some of his former graduate students and the polymer science faculty of the Chemistry Department, especially through the efforts of Mohan Srinivasarao, now on the faculty of Georgia Tech, received support from the Office of the Dean of the Mellon College of Science. The symposium was opened with the announcement by Dean Richard McCullough that Berry had been named a University Professor of Carnegie Mellon, and the lecture sessions were closed with the presentation by Chemistry Department Head Hyung J. Kim of a 150 year old Ponderosa Pine bonsai to Berry (he immediately turned the surprise gift over to his wife Marilyn for her expert care!). The symposium included speakers from the local scene, as well as from polymer science programs from around the US (including one scientist from Japan, who happened to be visiting in the US at the time). The participants were treated to a cruise on the three rivers by the Gateway Clipper fleet, before the meeting closed with a poster session highlighting the diverse research in polymer science at Carnegie Mellon.



Some of the Symposium participants on the steps of MI during a break: GCB (center) talking with Dick Stein, Marilyn Berry (right) with Kris Matyjaszewski, and Mohan Srinivasarao with Jung -Ok Park (foreground), two of the four former GCB grad students in the photo.

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### Terrence J. Collins (Continued from page 4)

chemistry over the last 20 years at Carnegie Mellon. The Collins group, which specializes in inorganic and green chemistry, has developed a family of environmentally friendly oxidation catalysts that can be applied to a diverse range of industrial and public health problems. These innovative catalysts, which are shown in the figure, have iron in the center of a specially designed ligand framework. This ligand framework allows the iron center to react and activate hydrogen peroxide, a green oxidant, in a very efficient manner. Chemists have in the past prepared good oxidation catalysts but they did not survive for very long in the oxidizing conditions that they created. The Collins' catalysts solve the lifetime problem by using a ligand struc-

ture that essentially has no sites on it that are sensitive to oxidation. The catalysts are referred to as TAML<sup>®</sup> activators which reflects the tetra amido core that they are built upon.

While the fundamental kinetic and mechanistic aspects of how the TAML<sup>®</sup> activators function are still under investigation, application areas are already being pursued. One of the great appeals of the

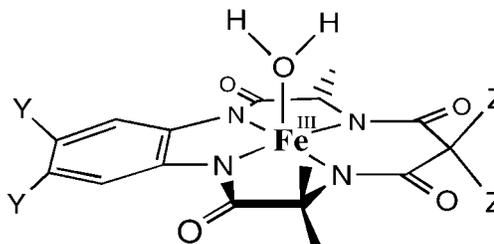


Professor Terry J. Collins (right) and Dean Richard D. McCullough on the occasion of Collins being named the Thomas Lord Professor of Chemistry in June 2002.

TAML<sup>®</sup> activators is that they function best in the part per million (ppm) range. Thus when they are used in large scale applications, only trace amounts are required. For example, field trials have been conducted on the treatment of the waste water

effluent from pulp and paper mills. Those living on a river downstream from a mill know how mill discharges discolor the river. This color has negative impacts on the biology of the river. The field trial was designed to determine how the TAML<sup>®</sup> activator could be used to decolorize a 6 million liter per day effluent stream. By taking a portion of the effluent and running the trial for two weeks, it was found that 1 ppm of the TAML<sup>®</sup> activator reduced the color by almost 80% in less than one hour. This translates into 6 kg of TAML<sup>®</sup> activator to treat 6 million liters of waste. There is no other technology that can do this as efficiently. We have other examples where the TAML<sup>®</sup> activators and hydrogen peroxide, provide new opportunities for industry to solve some of their most challenging problems. These can be found at the Collins group website along with the many other areas of chemistry being pursued:

<http://www.cmu.edu/instituteforgreenoxidationchemistry/>



An example of a TAML<sup>®</sup> activator

The Collins' team of 15 investigators operates out of the Institute for Green Oxidation Chemistry on the CMU campus. Collins' work was recognized in 1999 by the *Presidential Green Chemistry Challenge Award* (USA) and in 1998 by the *Award of the Society of Pure and Applied Coordination Chemistry* (Japan). Professor Collins is a Dreyfus Teacher-Scholar and a Fellow of the Alfred P. Sloan Foundation.

## Faculty Profiles *(Continued from p. 2)*

### Karen Stump *(Continued)*

Presidents (Mehrabian and Cohon). Karen Stump has been at the project's core from beginning to end, as Chemistry's departmental liaison and a member of the Executive Committee for the building project. Karen has been called upon for myriad design decisions about the labs that used her detailed knowledge of the current educational programs and her creativity for future courses in the state-of-the-art "megablab," such as new curriculum for interdisciplinary learning spaces. She never lost sight of the fact that great space attracts great students and enhances their learning opportunities in innumerable ways.

Among the many decisions concerning the new laboratories, she kept safety as a priority, supervising decisions about air handling, safety showers, chemical storage facilities, and factors affecting lines of sight for instructors. Her emphasis on safety led her to create and present a new mini-course for sophomore chemists, taught for the first time in Spring 2002. The course utilizes a series of lab explorations, projects, and guest lectures on key topics such as hazardous materials, toxic waste, OSHA lab standards, and common lab emergencies. Her interests in excellence in laboratory instruction and safety have motivated her development of a mentoring program for graduate student Teaching Assistants, with over 12 hours of sessions to better prepare TA's for their roles in teaching undergraduates as instructors in recitation or laboratory, or as graders.

Beyond Carnegie Mellon, Karen has also made important contributions to K-12 education through a wide variety of outreach programs for students and teachers. Most recently, she received state funding for a five-year Governor's Institute for Physical Science Educators that brings 40-50 teachers to Carnegie Mellon for a two-week intensive summer program. Her dedication to teaching at all levels was recognized by the regional 2002 *Responsible Care Catalyst Award* from the American Chemistry Council. The Award honors teaching excellence among college and university teachers.

### Garry Warnock *(Continued)*

Society of Chemistry of Pittsburgh. In addition, the program received a grant from the Society for Analytical Chemistry of Pittsburgh and, most recently, a generous contribution from Mark Gelfand. This support has allowed the Science Workshops for teachers, held in the Mellon Institute, and numerous Teacher In-Service Day programs organized for the Pittsburgh Public Schools. In addition, the team has developed a highly active and dynamic relationship between the CMU Science Van team and teachers and students from several regional school districts, including the Pittsburgh Public School district. In addition to Warnock, the Outreach team is composed of three master teachers, Hugh Carr, John Ziegler and Ed Schrothe, who themselves had highly successful careers in area high schools; Mount Lebanon,

Riverview and Quaker Valley, respectively. Their continued vision, energy and goodwill has created an outreach program that has earned enthusiastic praise for all its efforts on behalf of area students and teachers.

To date the program has impacted scores of teachers and hundreds of students. Its multi-faceted approach is designed to engage all participants at several levels. The team brings "hands-on" science experiments into the classroom to allow all students the opportunity to experience scientific experimentation and they present Science Shows to large student audiences. More than seventy Saturday Science Workshops for teachers have been held in the Mellon Institute. In addition, the team annually presents to the Pittsburgh Conference, which this year will be held in Orlando. Every Spring they are invited to contribute to the "Focus on Spectroscopy", a series of presentations for Middle School students held at the Carnegie Science Center.

You can learn more about the Van-Outreach program from their web site at the url:

<http://www.cmu.edu/mcs/van-outreach>

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## A Siloxane Connection

Perhaps all of you are aware that Carnegie Mellon was formed in the mid '60s by the merger of Carnegie Institute of Technology (CIT) with the Mellon Institute (MI). You may not realize that the two institutions had many connections prior to the merger, including joint appointments held by John A. Pople, later recognized for his work in theoretical chemistry with a Nobel Prize (1988). The obituary notice for Carnegie Mellon alum Earl Warrick elsewhere in this issue brings to mind an important connection from the late '40s and early '50s: Warrick was working on his D.Sc. in Chemistry at CIT under Paul Fugassi in that period, while working at MI for the Corning Fellowship. The group at MI was charged to investigate silicon chemistry of potential interest to Corning, particularly potential adhesives and other polymeric materials. That effort was stunningly successful. Similar studies



Earl Warrick (rolled-up sleeves) with colleagues in his MI research lab, circa '40s.

ongoing at Dow Chemical in Midland, MI, motivated Dow and Corning to create a new company based on the research developments in silicone chemistry in the two research laboratories, the Dow Corning Company, with its research arm in the Dow Corning Fellowship at MI. The urgent needs of the military in the '40s provided ample opportunities to develop a market for the new materials, which filled many important niches. The work on siloxane chemistry continued in the MI Fellowship through 1956, at which time it was moved to new facilities of Dow Corning in Midland, MI. Along the way, Warrick noticed the peculiar properties of a polysiloxane compounded with a filler, which he dubbed a "bouncing putty". Interesting enough for a patent, but with no apparent technological application, the material was put aside. Only later was the material marketed under the name *Silly Putty*, to the delight of many a child (and some adults too!). A much more complete rendition of this history may be found in the book *Forty Years of Firsts: The Recollections of a Dow Corning Pioneer*, written by Earl Warrick (McGraw Hill, 1990).

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## Research Profiles

**David Yaron** and his research group are working to devise models to describe the electronic properties of conjugated polymers, a class of materials that has great potential for electronic and photophysical applications such as flat-screen displays and organic transistors. His research group is developing new approaches to modeling the excited electronic states that mediate the photophysical processes occurring in these materials. Describing these excited states poses interesting and challenging problems in the electronic structure theory of large systems. Much of their recent effort has gone into developing methods that can describe the effects of disorder, such as non-uniform morphologies and chemical defects, on the photophysics. Understanding the effects of disorder is crucial to improving the performance of devices based on these materials.

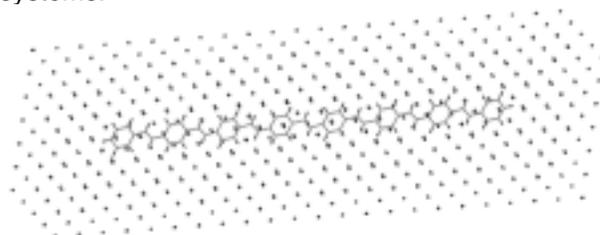
Since it is difficult to obtain either a purely experimental or theoretical handle on the nature and magnitude of disorder, Yaron's group has teamed with Linda Peteanu in a joint experimental/theoretical effort. The electroabsorption spectra collected in Linda Peteanu's group yield the change in the dipole moment,  $D_m$ , and polarizability,  $D_a$ , accompanying electronic excitation of conjugated polymers and oligomers. Due to the centro-symmetric chemical structure,  $D_m$  should be zero for an ordered solid. However, substantial  $D_m$ 's are seen experimentally and these provide an experimental handle on the degree of disorder in the system. Borrowing language from electron-transfer theory, they have defined two types of disorder in these systems:

**Inner-sphere disorder** arises from distortions of the molecule away from the ideal centro-symmetric structure. These are modeled by generating an ensemble of structures, typically focusing on the torsional

degrees of freedom since these are low-energy motions that are strongly coupled to the disorder of the side-chains.

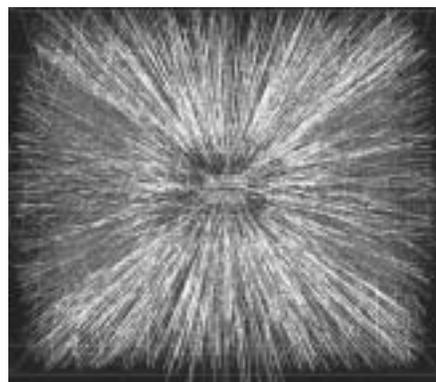
**Outer-sphere disorder** arises from the amorphous nature of the surroundings, which are currently modeled via a lattice of random dipoles such as that shown in the figure below.

In poly(paraphenylenevinylene) (PPV), an important material for photophysical applications such as flat screen displays, both types of disorder contribute significantly to the breaking of centrosymmetry. By combining electroabsorption experiments with theoretical modeling, they have been able to quantify the degree of structural and environmental disorder in these systems.



*The effects of environmental disorder are modeled by placing a PPV oligomer in an array of randomly-oriented dipoles.*

**Mort Kaplan** and his research group are actively involved in the multinational STAR Experiment, the goal of which is to recreate and study the primordial chemistry of the very early universe. Using the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory – the world's newest and largest particle accelerator for nuclear research – beams of gold ions are smashed into each other at very high energies, in order to produce an elusive form of hot, dense matter called "quark-gluon plasma", thought to have last existed just an instant after the "big bang" birth of our universe. The STAR Detector, a very large electronic 3-dimensional camera, captures the transient states of matter. The figure below displays a "picture" of a single collision event, showing tracks of the many particles produced in the collisions, and provides the signatures reflecting the several thousand tracks can be seen radiating outwards from



*Image of tracks produced in a single collision event*

the central collision zone. Although the experiment is still in its infancy, there is already very strong evidence that the collisions have yielded matter densities many times greater than normal nuclear density, with associated temperatures more than seven billion times room temperature. As new data continues to be collected, the challenge of unraveling and interpreting the complex phenomena is well underway, resulting in more than 25 journal publications and Conference Proceedings in calendar 2002.

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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—please keep them coming! As usual, capsules from your questionnaire responses are included below.

### Earl L. Warrick

BS '33; MS '34; DSc '43, died at age 91 on November 22, 2002. He was a Chemistry alum and a research scientist with Industrial Fellowships at Mellon Institute '35 to '56, before moving to Dow Corning in Midland, MI. He received an Alumni Merit Award from Carnegie Mellon in 1976, the year of his retirement from Dow Corning. He also received the Charles Goodyear Medal from the American Chemical Society that year. He subsequently was affiliated with Saginaw Valley State College in Michigan. Further remarks on his career may be found elsewhere in this issue.

### Jay J. Lindsay

PhD '74, passed away December 25, 2001 in his home. He is survived by his wife of 31 years, Charlene Weekly Lindsey, and 2 daughters. Most recently, Dr. Lindsey was the Vice President of Business Planning/Technology at Rhein Chemie Corporation, a subsidiary of Bayer Corporation in Trenton, NJ.

**Fred S. Karn**, BS39, studied chemistry under Dr. Warner. He worked in petroleum chemistry in New York with Standard Oil; coal chemistry in Pittsburgh with Bu Mines, Department of Energy, and studied catalysis of synthetic fuels.

**Robert L. Marcus**, BS45, entered medical school in September 1945 after completing 3 years at Carnegie Tech. He did not get a degree at Carnegie Tech, but did get an M.D. degree from what is now Case Western Reserve School of Medicine in June 1946. Dr. Marcus has been in the private practice of medicine with his specialty being psychiatry since June 1953. His wife is a full professor in the School of Social Welfare at the State University of New York at Stony Brook. They have two children. Their son is a mathematician

and is working in private industry. Their daughter has an MBA, works part-time, and has four children, ages 7 to 13.

**Carl E. Sherrick**, BS48, is now retired from research and teaching at Princeton University (experimental psychology). He has three daughters, all married, and three grandchildren. He is now widowed and living alone in Bucks County, finding lots of new things to do in a very pleasant part of Pennsylvania. He sends his best wishes to the Department and to fellow alumni.

**Arnold E. Reif**, MS49/DSc50, is a Research Professor of Pathology, Emeritus, at Boston University School of Medicine, where he was Chief of the Laboratory of Experimental Cancer Immunotherapy at the Mallory Institute of Pathology. Dr. Reif also holds an M.T.S. degree from the Divinity School, Harvard University, Cambridge, MA since 1993.

**Richard J. Windgassen**, BS55, writes "I was quite surprised to read in the January, 2002 "Carnegie Mellon Chemist" that the average time for earning a PhD was 5.5 years. Back in 1958, a PhD in Organic Chemistry could be earned in as little as three years (four was stretching it). And those were the days before NMR analysis and even gas chromatography. I know there is more to learn these days, but there are also super tools to work with. In 1958 an article appeared arguing that in less than 50 years, the prospective PhD would check a computer, select his thesis topic, supply his name and school for the title page, and the computer would do the work and print the thesis. Like on-time aircraft at airports, here's another technology that never materialized. The delay for PhD has actually increased, with the doctorate being further delayed to 5.5 years.

**Marilyn Casey Bracken**, BS57, is President, Bracken Associates. Before starting her own firm, Dr. Bracken was President of Paragon Global Services and Vice President, Marketing and Business Development of the Environmental Sciences Group of Applied Bioscience International, Inc. Earlier, she was Senior Vice President, Federal Programs, Air & Water Technologies.

**Gary J. Long**, BS64, is Professor, Department of Chemistry, University of Missouri-Rolla. He received the prestigious Belgian appointment as the "Chaire Francqui Interuniversitaire au titre étranger," or the International Francqui Chair, for the 2002-2003 academic year. His nomination for this chair was based on his internationally recognized achievements in Mössbauer spectroscopy and was supported by six Belgian universities. Although the University of Liege will serve as the host university, Professor Long will lecture on his scientific work at all six universities. Further, the University of Liege will organize an international symposium on materials science in honor of Professor Long near the end of his professorship, which is tentatively scheduled for January to June 2003.

**Vince Sullivan**, PhD90, did a three year assignment in Germany while working for Hoechst Celanese. He returned to the US in 1999 and shortly afterwards went to work for Becton Dickinson, a medi-

cal device manufacturer. He's been working at their North Carolina division for the last 3 years and enjoys being involved with more technical work. His group is working on novel drug delivery devices and formulations; everything from materials to microbiology.

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### The Departmental Web Site

Regular improvements and additions to the department web site continue. The graduate student section has been reorganized to better meet the needs of prospective students. Research group sites continue to be updated, including a new site for the Achim, Bier, Matyjaszewski and Llinas groups. The CMA and Science Van Outreach site is also new. A new module will also soon be available on the ACS web site that features work by Terry Collins on sustainability ethics. The Interdisciplinary Undergraduate Science Laboratories site (<http://www.cmu.edu/mcs/uglabs>) has photos of the construction and completed rooms, in addition to photos from the October 4 grand opening celebration. 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](mailto:rf51@andrew.cmu.edu), and visit us at the url:  
<http://www.chem.cmu.edu>

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### THANKS FOR YOUR SUPPORT!

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## 2003 ALUMNI QUESTIONNAIRE

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Yes

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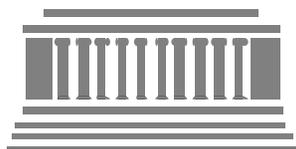
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