The Graduate Alumni Newsletter
of the Department of Chemistry
at Cornell University and the
Society of Cornell Chemists

Cornell Chemistry Research

March 1990
Issue 46

Molecular Modeling

Graduate students in chemistry are taking a new course in molecular modeling taught by Professor Charles F. Wilcox.

Many different computer packages are being run on Hewlett Packard Vectra ES12 workstations. For example, using *PC Model* software by Serena, students analyze and predict the properties of many different molecules. A Kodak DataShow 480 Projection Pad projects the computer-generated image to a large screen in the front of the classroom. As data points are selected and computations are done, all the students can see the process. Later, they use the same software to do similar analyses themselves.

"Modeling is a way of explaining molecules, and leads to the ability to predict new behaviors of molecules," commented Wilcox. "If one defines molecular modeling as mimicking the behavior of molecules, the physical properties, shapes, and chemical behavior, then chemists have been modeling molecules all along. Some chemists use a physical mode, like ball and stick models, some use more abstract modes, such as mathematics or equations, and now we are using visual images on the computer screen."

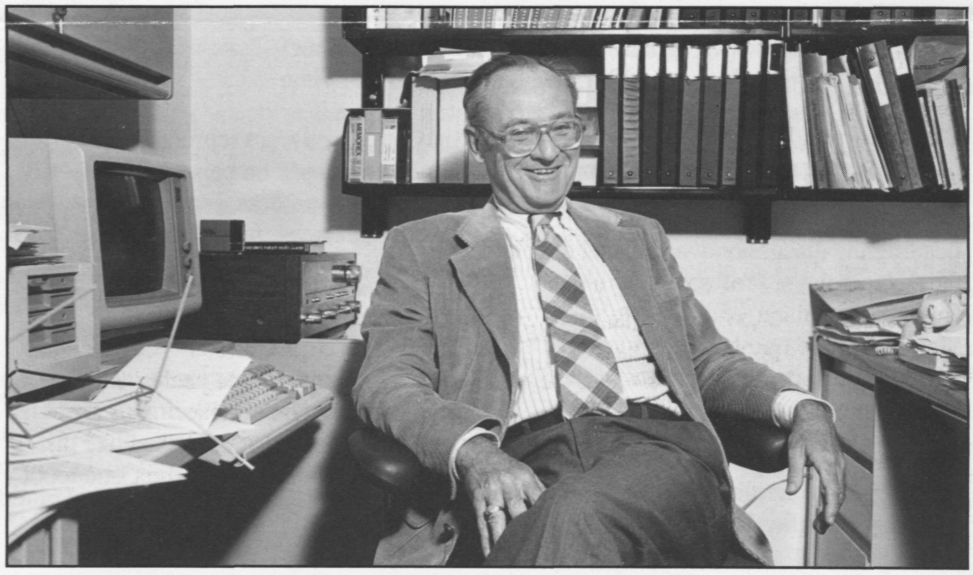
More and more researchers in industry are expected to know how to use computers as research tools; it is important that graduate chemistry students acquire facility using those new tools before they begin their professional research careers.

The department received 12 HP Vectras as part of a $160,000 grant from Hewlett Packard, and one of the machines was committed to the development of molecular modeling curriculum for inclusion in a graduate chemistry course. Wilcox developed an instructional plan to be incorporated in the graduate-level physical organic chemistry course he taught in the fall of 1989.

Computer modeling can be more accurate than other forms of modeling, and is certainly more flexible. In the classroom, the dynamic images on the screen engage the students more effectively than chalk drawings or transparencies. The biggest advantage, however, may be that the computer-generated images encourage "what if" discussions during which the students propose variations in the data and can observe the calculations and the results taking shape on the screen.

A new computer graphics facility being planned for Baker Lab will house computers networked through the Chemistry Research Computing Facility to the Cornell Supercomputer Facility. That will provide more power for faster calculations and for more sophisticated data analysis.

"Eventually," said Professor Wilcox, "I hope we'll get a computer and a state-of-the-art audio-visual system permanently installed in one of the lecture rooms."



Professor Charles F. Wilcox

Spring Lecture Series

Baker Lectures

John S. Waugh, Institute Professor at MIT, will be the 1989-90 George Fisher Baker Lecturer in the Department of Chemistry.

The ten lectures, which will cover various topics in Nuclear Magnetic Resonance, will begin on March 27.

Waugh has received the Langmuir Award in chemical physics, the Pittsburgh Award in spectroscopy, the Pauling Medal, the Wolf Prize, and the ISMAR prize in magnetic resonance. In 1987 he was awarded the Distinguished Alumni Award by CalTech, where he received his PhD in chemistry and physics in 1953. MIT honored him with its Killian faculty achievement award in 1988, and in 1989 he received the ScD (Honoris Causa) from Dartmouth College, where he earned his AB in 1949.

The George Fisher Baker Lecture series was established in 1926 at the suggestion of L.M. Dennis, then the chairman of the Department of Chemistry, to invite the most eminent chemists of the world to lecture at Cornell. Mr. Baker, who had given 1.5 million dollars toward the construction of a new chemistry laboratory in 1920, donated a further $250,000 to be used for the lecture series.

Of the 77 lecturers in the series (no lectures were held from 1940 - 1947), 19 have become Nobel Laureates.

Bayer/Mobay Lectures

C. Grant Willson, the 1989-90 Bayer/Mobay Lecturer, is manager of Polymer Science and Technology at the IBM Almaden Research Center. The lectures given on January 29, 30 and February 1, were entitled "Organic and Polymer Chemistry in the Microelectronics Industry," "Polymers as Imaging Materials for Microlithography," and "Organic Materials for Non-Linear Optics."

Since joining IBM in 1978, Dr. Willson has reached the seventh level of patent achievement award and has received six outstanding innovation awards from IBM for his work with novel polymers for micro-electronics. Appointed an IBM Fellow in 1985, he is currently the only chemist within IBM to hold this highest corporate scientific distinction. In 1986, Dr. Willson received the Arthur K. Doolittle Award from the American Chemical Society, Division of Polymeric Materials: Science and Engineering. He received the Humboldt Senior Scientist Award for 1988-89.

The Bayer/Mobay Lecture Series is sponsored annually by the Mobay Corporation, a Pittsburgh-based manufacturer of polyurethane materials, and by Bayer AG, the West German chemical and pharmaceutical concern.

Debye Lectures

The 1989-90 Debye Lectures were given by Professor Mark Wightman, the W. R. Kenan, Jr. Professor of Chemistry at the University of North Carolina.

The three lectures, entitled "Electrochemistry in Small Domains," "Biosensors for Catecholamines," and "Voltammetry Under Unusual Conditions," were given on February 20, 21 and 22 in room 119 Baker Laboratory.

Professor Wightman, who earned his PhD in 1974 from the University of North Carolina at Chapel Hill, was a member of the chemistry faculty at Indiana University from 1976 to 1989. During that time he received the National Institutes of Health Research Career Development Award (1979-1983), the Alfred P. Sloan Fellowship (1981-83), and the NIH Jacob Javits Neuroscience Investigator Award (1988).

He is on the Board of Directors of the Society for Electroanalytical Chemistry and is a member of the Electrochemical Society, the American Chemical Society, and the Society for Neuroscience.

The Debye Lecture Series, established in 1963, is sponsored by the American Chemical Society, and honors the late Peter J.W. Debye.

Panel Discussion on Ethics

Chemistry faculty and graduate students participated in a discussion of scientific integrity held in Baker Lab in mid-January.

Leading the discussion was a panel of four faculty members, Professors Abruña, Collum, Hoffmann, and Meinwald. Moderating the two-hour session was Dr. Earl Peters, Executive Director of the department.

Each panel member used anecdotes and hypothetical examples to illustrate points of ethics and integrity in scientific research.

Subjects raised were reproduceability, appropriate credit on papers, the integrity of the review process, settings under which fraud is enhanced, formal university procedures for dealing with fraud, and what to do if you think there is sloppy or even fraudulent research going on.

Jon Clardy, department chair, instituted the discussion session after seeing the booklet, *On Being a Scientist*, published late last year by the Committee on the Conduct of Science, National Academy of Sciences.

ACS Meeting

The 199th ACS National Meeting will be held April 22-27 in Boston. Cornell Chemistry will be holding a continental breakfast on Tuesday, April 24. Check the February 26 issue of *Chemical & Engineering News* for more details and ticket information.

Faculty News

Andreas C. Albrecht has been awarded the 1990 Earle K. Plyler Prize of the American Physical Society, sponsored by the George E. Crouch Foundation. The prize recognizes and encourages notable contributions to molecular spectroscopy. Professor Albrecht received the prize "for his fundamental experimental and theoretical contributions to condensed phase molecular spectroscopy, encompassing time-resolved Raman spectroscopy, the exploitation of photoselection by absorption of polarized light, multiphoton excitation and ionization in condensed phases, and local-mode behavior in large molecules."

Paul L. Houston has been elected a Fellow of the American Physical Society. He was selected "for important contributions toward understanding molecular photodissociation dynamics, energy transfer, and gas-solid interactions; in particular, for his imaginative use of photofragment imaging and his development of the field of vector correlations."

Atsuo Kuki is one of fourteen young chemistry faculty members nationwide to receive the 1989 Camille and Henry Dreyfus Teacher-Scholar award. The award confers an unrestricted grant of $50,000 for support of Kuki's professional activities. Winners of the award are within the first five years of their first full-time academic appointments.

Professor emeritus **Frank A. Long**, who is now at the School of Social Sciences at the University of California at Irvine, has been awarded the 1989 AAAS Philip Hauge Abelson Prize. The award is given annually to "a scientist whose career has been distinguished for both scientific achievement and for other notable services to the scientific community." Professor Long is well known for his research in physical chemistry and for his contributions to solving major world problems including international security, science policy, and third world development.

Harold A. Scheraga is the 1990 recipient of the American Chemical Society award in Polymer Chemistry, which is sponsored by the Mobil Chemical Company. The honor has been conferred for "his innovative application of polymer principles to elucidating the conformational properties of polypeptides and other macromolecules." Professor Scheraga has also been named to receive the 1990 ACS Biological Chemistry Division Repligen Award, for numerous contributions in the area of physical chemistry of proteins, including applying polymer principles to the elucidation of the conformational properties of polypeptides and other macromolecules. Both awards will be presented at the April ACS meeting in Boston.

Ben Widom will be a Fulbright Scholar during the spring semester, 1990. He'll be doing research on the theory of polymers and polymer solutions, in the group of P.G. de Gennes at the Ecole Supérieure de Physique et de Chimie Industrielles

Alumni News

Stuart Baum, PhD 65, was one of only thirteen people statewide named distinguished teaching professors by the State University of New York Board of Trustees in 1989. Faculty members named distinguished teaching professors must "perform superbly in the classroom, provide academic advisement, maintain high standards of student performance, and continue to be an active scholar." Baum, who worked in the research group of Bob Plane here at Cornell, has taught at SUNY Plattsburgh since 1965. He writes that his son, Derek, graduated from the Hotel School in 1988, and his daughter, Kym Michelle, is a senior in the School of Human Ecology.

Laurence E. Fried, PhD 88, and **Evan R. Williams**, PhD 89, were among eighteen young scientists selected in 1989 by the National Science Foundation to be Postdoctoral Research Fellows in Chemistry. Fried, who worked with Greg Ezra here at Cornell, is now a postdoctoral associate with Shaul Mukamel at the University of Rochester. Williams has been a member of Fred W. McLafferty's research group while at Cornell, and will join Dick Zare's group at Stanford University.

Alumnus Establishes New Prize

Leo Mandelkern, AB '42, PhD '49, and his wife, Berdie, have established a new prize for "an outstanding student enrolled at Cornell University in its College of Arts and Sciences who is a senior majoring in chemistry, has excelled academically and will go on to graduate study in chemistry or biochemistry." The Leo and Berdie Mandelkern Prize will be awarded for the first time in June 1991, and annually thereafter.

Mandelkern spent 49 months in the army after earning his AB in chemistry at Cornell in 1942, and returned to Cornell as a member of Professor Frank Long's research group. He received his PhD in chemistry here in 1949. From 1949 through 1951, he was a postdoctoral associate with Paul Flory. He was a visiting professor at Cornell during the spring of 1967.

During his long and productive career, Mandelkern has been active in research on the physical chemistry of high polymers as well as biophysics and macromolecules. He was a physical chemist at the National Bureau of Standards from 1952 to 1962, and then joined the faculty at Florida State University, where he is the R. O. Lawton Distinguished Professor of Chemistry. He received the Fleming Award in 1959, the Polymer Chemistry Award of the American Chemical Society in 1975, the Mettler Award of the North American Thermal Analysis Society in 1984, the George S. Whitby Award of the Rubber Division of the ACS in 1988, and the ACS award in Applied Polymer Science in 1989.

Dr. and Mrs. Mandelkern's generous gift is an important factor in encouraging our most talented and dedicated students to pursue careers in scientific research, and we are most grateful.

Letter from the Chairman

One of the most important jobs facing the department is the task of renewing itself through the appointment of new faculty members. While appointments have always been formidable propositions, they are even more challenging today. The number of Ph.D.'s interested in academic careers is declining, and the cost of setting up ever more sophisticated laboratories is rapidly escalating. Due to retirements and departures, the department is faced with making an appointment every year for the foreseeable future in order to maintain our current size.

The Cornell Chemistry Department has just successfully finished a search for an analytical chemist, and I'm delighted to report that Dr. David B. Zax will be joining us in August. You will read more about David in a future issue. He's coming to Cornell from the Weizmann Institute where he's been working following postdoctoral work at the University of Illinois, Ph.D. work at Berkeley and an undergraduate degree at Harvard. David is an expert in modern NMR techniques, especially solid state NMR. We've long recognized NMR as a crucial need for the department and are delighted that someone with David's outstanding record and promise will be here.

One of the most gratifying jobs to me as Chair is watching younger faculty launch academic careers. I'd like to make special mention of Atsuo Kuki who was just selected as one of the 1989 Camille and Henry Dreyfus Teacher-Scholar grant awardees. Nominations for these prestigious grants are limited to one per university, and only fourteen winners are selected nationwide. Congratulations Atsuo.

You might have noticed a subtle change in the heading of Cornell Chemistry; the issue you received was designated as either the "graduate" or "undergraduate" alumni newsletter. We made this change so that the newsletter would be more appropriate for our (slightly) different constituencies. If you'd like to receive both, just let us know.

-Jon Clardy

Cornell Chemistry is published by the Department of Chemistry at Cornell University.
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