

# **Department of Chemistry**

Alumni Newsletter – Fall 2008



**Work has begun**  
Construction is under way on Hach Hall

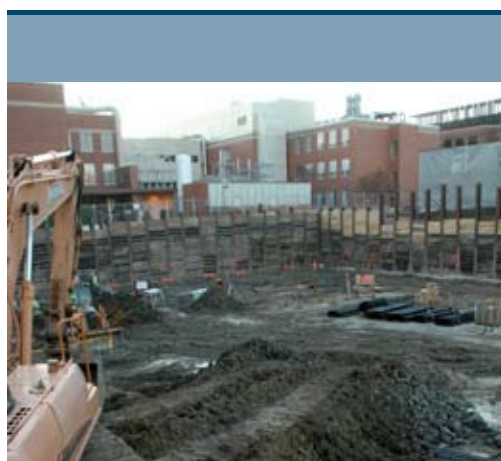
**IOWA STATE UNIVERSITY**  
College of Liberal Arts and Sciences

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The newsletter is published once a year for the alumni, friends, students and faculty of the Department of Chemistry at Iowa State University, an academic department in the College of Liberal Arts and Sciences.

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**On the cover**

Hach Hall construction begins. View the progress online:  
[www.fpm.iastate.edu/webcam/chemistry/](http://www.fpm.iastate.edu/webcam/chemistry/)  
 Photo by Dave Gieseke

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## Features

### 7 A Rich background in chemistry

Alumnus Jonathan Rich is a silicone chemist. He can trace his roots back to the first chemistry class he took at Iowa State.

### 8 Construction is under way

By the time the ceremonial groundbreaking took place, workers had already begun working on the Department of Chemistry's new building, Hach Hall.

### 11 Giving to Iowa State's need

Gene Lange is not a chemistry grad, but the Iowa State alumnus wanted to ensure his gift had a sizeable impact on the campus.

### 12 AAAS Fellow

Solid state chemist Gordon Miller was named a prestigious AAAS fellow.

### 13 PIRE initiatives

Faculty member Theresa Windus aspires to promote NSF international research effort.



Dear Friends of Chemistry and Iowa State University,

This fall semester began in the most beautiful way possible. On a beautiful Saturday morning on 6 September, as the Iowa State University marching band broke into a fanfare, we ceremonially broke ground for the new chemistry facility, Hach Hall. We could not have arrived at this momentous occasion without the support of the friends, faculty, and staff of the Department of Chemistry; the State of Iowa; the Roy J. Carver Charitable Trust; and, of course, the generous gift of Mrs. Kathryn Hach Darrow and the Hach family.

You can monitor the progress of the construction of Hach Hall by using the following link to our live webcam: <http://www.fpm.iastate.edu/webcam/chemistry/>. President Geoffroy has indicated that he expects the Hach Hall to be occupied in 2010.

This fall, we welcome three new faculty to our ranks. Tom Holme comes to us as a Full Professor in the areas of chemical education and computational physical chemistry. Tom brings the American Chemical Society Examinations Institute with him. The Institute is responsible for generating all the ACS standardized chemistry examinations that are used at the high school and university levels. Ning Fang and Young-Jin Lee join us as Assistant Professors in the area of analytical chemistry. Ning is an expert in single-molecule spectroscopy; and Young-Jin is an expert in mass spectroscopy.

We are fortunate to have support from President Geoffroy to continue his Presidential Lecturer series. Our fourth Presidential Lecture will be given on Tuesday, 31, March 2009 by Professor Dudley R. Herschbach, the Frank B. Baird, Jr., Professor of Science at Harvard and recipient of the 1986 Nobel Prize in chemistry.

Finally, for the third year in a row, I have had the honor of accompanying our undergraduate Hach Scholars to Ft. Collins, Colorado to attend a reception and banquet hosted by the Hach Scientific Foundation. The keynote speaker at this year's banquet is Carl Wieman, 1995 Nobel Laureate in Physics.

If you have the opportunity to visit Ames, please stop by the Department. I welcome the occasion of meeting you and of showing you and talking to you about the exciting developments Chemistry is undergoing.

Yours sincerely,

Jacob W. Petrich  
 Professor and Chair

## Chemistry's Patricia Thiel receives Iota Sigma Pi honor

Patricia Thiel, Distinguished Professor in Liberal Arts and Sciences and professor of chemistry at Iowa State University, has received the highest honor bestowed by Iota Sigma Pi, the national honor society of women in chemistry.

This award, named the National Honorary Member Award, is "for exceptional and significant achievement in chemistry or an allied field of such nature as to merit international recognition." It is given to only one person every three years.

An expert in the chemistry and physics of surfaces, Thiel has made pioneering contributions in three main areas: surfaces of quasicrystals, interactions of water molecules with metal surfaces, and the evolution and growth mechanisms of metal nanostructures.

She has served on the Committee of Visitors for the Division of Chemistry of the National Science Foundation (NSF) and has been a member of the advisory council of the Office of Basic Energy Sciences for the U.S. Department of Energy (DOE). At Iowa State, Thiel formerly served as director of the Materials Chemistry Program of the U.S. Department of Energy's Ames Laboratory and as chair of the Department of Chemistry.

Her numerous awards and honors include the NSF Presidential Young Investigator Award, the ISU Foundation Award for Outstanding Achievement in Research and the DOE's Award for Outstanding Scientific Accomplishment

in Materials Chemistry.

She is a Fellow of the American Physical Society, American Vacuum Society and the Institute of Physics.



## New faculty join chemistry staff

Three new faculty members have joined the Department of Chemistry faculty in time for the 2008 fall semester:

Thomas Holme, professor, joins the faculty from the University of Wisconsin-Milwaukee where he worked for a number of years. A 1987 Ph.D. from Rice University, Holme's area of expertise includes chemistry education and computational chemistry.

Ning Fang, assistant professor, was previously a post-doc fellow at both Iowa State and the U.S. Department of Energy Ames Laboratory. He received a Ph.D. from the University of British Columbia in 2006 and specializes in bioanalytical and biophysical chemistry.

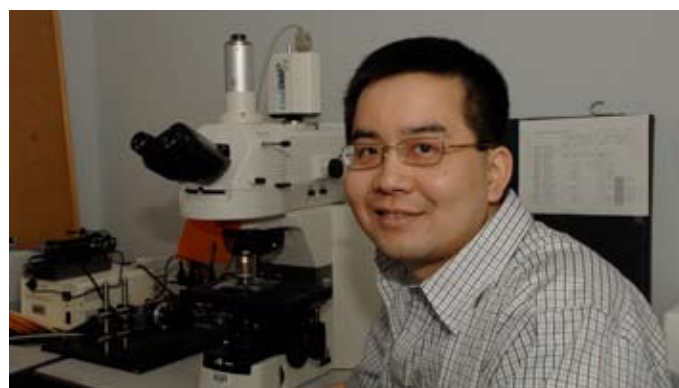
Young-Jin Lee, assistant professor, who holds a Ph.D. from Seoul National University in 1997. He studies biological mass spectrometry, proteomics and metabolomics. He was previously a mass spectrometry specialist at the University of California-Davis Spectrometry Center.



Holme



Lee



Fang

## Iowa State researchers develop technology for early detection of viruses

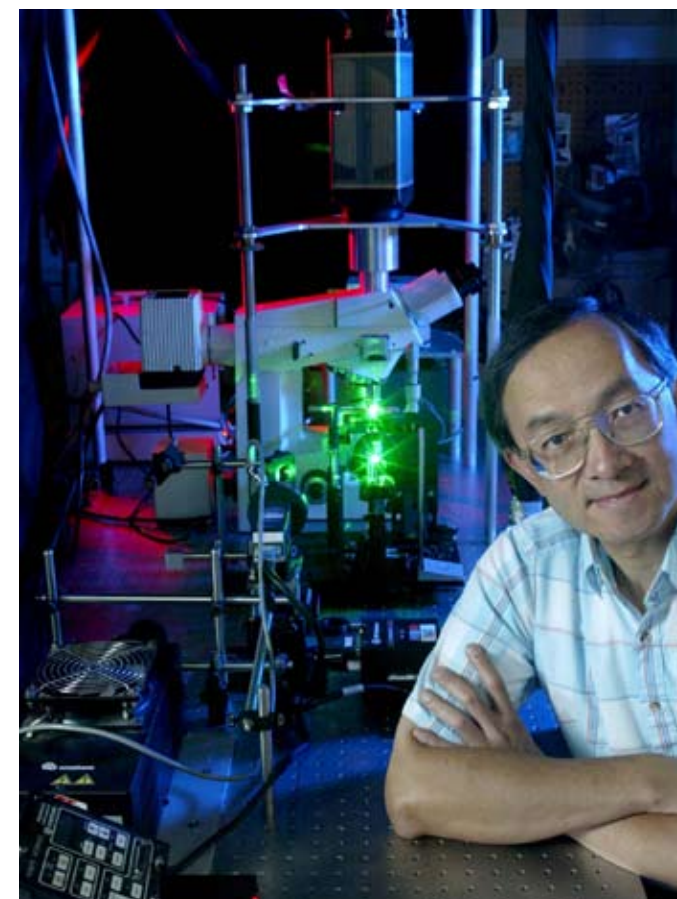
Iowa State researchers have developed a technology that detects a single molecule of the virus associated with cervical cancer in women.

That's a significant improvement over the current test for the human papillomavirus, said Edward Yeung, Distinguished Professor and the Robert Allen Wright Chair in Chemistry who led the research team that developed the new test. The current test, the Nobel Prize-winning polymerase chain reaction technique, requires 10 to 50 virus molecules for detection.

"We are always interested in detecting smaller and smaller amounts of material at lower and lower concentrations," Yeung said. "Detecting lower levels means earlier diagnosis."

The discovery by Yeung, who's also a senior chemist and deputy program director for the U.S. Department of Energy's Ames Laboratory at Iowa State; Jiangwei Li, an Iowa State doctoral student; and Ji-Young Lee, a former Iowa State doctoral student; was published in the Nov. 1 issue of the journal *Analytical Chemistry*.

Their work was funded by a five-year, \$950,000 grant from the National Institutes of Health with additional support from The Robert Allen Wright Endowment for Excellence at Iowa State.



## Chemists track how drug changes, blocks flu virus

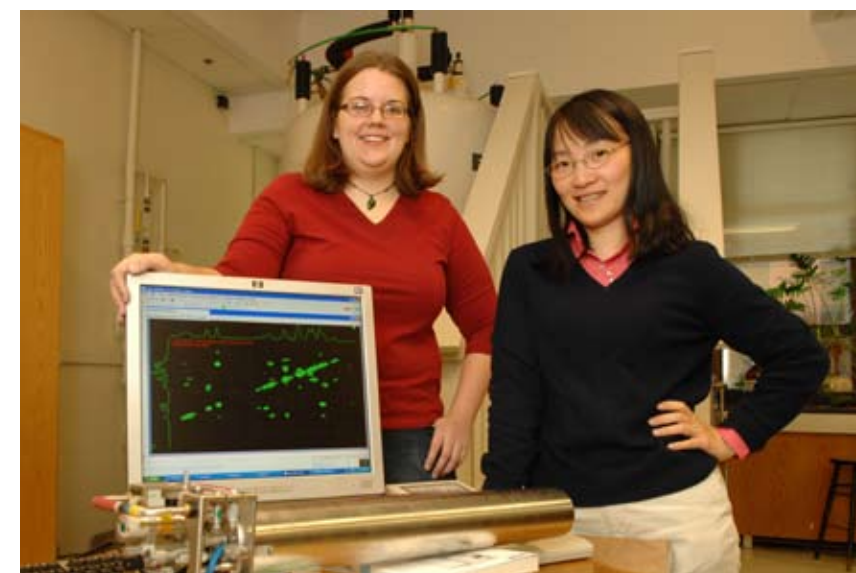
An anti-virus drug attacks influenza A by changing the motion and structure of a proton channel necessary for the virus to infect healthy cells, according to a recently published research paper by two Iowa State chemists.

Mei Hong, Iowa State's John D. Corbett Professor in Chemistry, and Sarah Cady, a graduate student in chemistry, are studying the effects of the antiviral drug amantadine on influenza A. That's the type of flu bug that most commonly makes people sick and the one that has caused the most serious flu epidemics.

Their findings appeared in the Feb. 5 edition of the *Proceedings of the National Academy of Sciences*.

Hong said the findings are particularly important because mutations of the type A virus are resistant to amantadine treatment.

"In the last few years, amantadine resistance has skyrocketed among influenza A viruses in Asia and North America, making it imperative to develop alternative antiviral drugs," Hong and Cady wrote in their paper.



Cady (left) and Hong

## Several faculty, staff receive college, university awards



Iowa State University and the College of Liberal Arts and Sciences have recognized several faculty and staff within the Department of Chemistry this past year.

### Recipients of Iowa State awards:

#### *ISU Award for Outstanding Achievement in Research* -

recognizes faculty members for outstanding achievement in research, scholarship, or creative activity.

(1) **John Verkade**, University professor. Verkade developed the novel chemical properties of his new phosphorus compounds, including their catalysis of important reactions. Several of these catalysts are now commercially manufactured. Some of his recent discoveries in phosphorus chemistry have become highly relevant to the production of value-added products from biomass and to recycling waste polyester fabrics.

#### *ISU Award for Mid-Career Achievement in Research* -

recognizes a faculty member who has demonstrated outstanding accomplishments in research at the mid-career stage.

(2) **Victor Lin**, professor. A world-renowned expert on the design of porous nanomaterials for selective catalysis and biotechnological/biomedical applications, Lin's research activities involve designing and developing novel strategies to control structure, morphology, biodegradability and function of these nanomaterials. His work has achieved significant impacts in the areas of drug-delivery and catalyst development for bio-renewable applications and bio-fuel production.

### Recipients of awards from the College of Liberal Arts and Sciences:

**Outstanding Teaching Award** - Recognizes faculty members for outstanding teaching performances over an extended period of time in undergraduate education.

(3) **Gordon Miller**, professor. In his 18 years at Iowa State, Miller has improved the student academic experience in chemistry at ISU and other campuses in the state. He has worked to improve safety in the lab and environmental responsibility and has increased opportunities for first-year undergraduates to become involved in research.

**Mid-Career Achievement in Research Award** - Recognizes faculty members who have a national or international reputation for outstanding contributions in research and/or artistic creativity at the mid-career stage.

(4) **Nicola Pohl**, associate professor. Pohl's research group is finding new ways to make and analyze sugars (carbohydrates) to dissect their important roles in plant, animal and human biology

and in biomass production. Her work serves as the basis for many collaborations with the College of Veterinary Medicine, the College of Agriculture and Life Sciences, the College of Engineering, Ames Laboratory, the National Animal Disease Center and many private industries.

#### *Ruth W. Swenson Award for Outstanding Advising Award*

- Recognizes outstanding performance as an undergraduate academic adviser over an extended period of time.

(5) **Walter Trahanovsky**, professor. Trahanovsky has been an outstanding adviser and mentor to ISU's undergraduate chemistry students for more than 44 years. He has been an active member of the American Chemical Society's Committee on Professional Training, which works to keep undergraduate curricula current.

#### *P&S Award for Excellence in Information Technology Award*

- Recognizes and honors Professional and Scientific employees working in the field of information technology who have demonstrated excellence in their position responsibilities.

(6) **Stephen Heideman**, teaching laboratory coordinator. In his role of Instructional and Administrative Computer Support, Heideman has been active in developing methods for isolating and securing computers interfaced with scientific instruments. He also built and maintains a web-based chemical inventory database for the chemistry teaching labs.

**Institutional Service Award** - Recognizes a member of the College of Liberal Arts and Sciences faculty for a history of exemplary institutional service that has benefited the department, college and/or the university.

(7) **Keith Woo**, professor. Woo has demonstrated a high degree of dedication and service to the Department of Chemistry and the university in his 22 years on campus. He has had oversight of the Chemical Instrumentation Facilities, is serving as the department associate chair and is chair of the new chemistry building committee.

**Merit Excellence Award** - Recognizes and honors Merit employees who have achieved excellence in their respective fields.

**Carolyn Marrujo de O'Hara**, secretary. This award is presented posthumously to de O'Hara, who died in September 2007. She joined the Department of Chemistry in 1999 and was known for her devotion to her colleagues and her work as well as her joyful personality, excellent skills and work ethic.

## A Rich background in chemistry



In his heart of hearts, Jonathan Rich ('77 chemistry) is a silicone chemist.

He can trace his roots back to the first chemistry class he took at Iowa State. And to the undergraduate research assistantship he had on campus with Tom Barton, now Distinguished Professor of chemistry.

Rich was in an organic chemistry class that Barton taught. Early in the fall semester, he went up to his professor.

"I asked him if he would be willing to take me in and let me assist him with his research," Rich recalled. "He could have dismissed me out of hand but instead he spent an entire afternoon with this sophomore chemistry major."

Barton gave Rich a job in his lab and the chemistry major worked the rest of his undergraduate years in the lab. The two remain in close contact to this day. Rich says it was that experience that made him aspire to become a silicone chemist.

After graduating with a Ph.D. from the University of Wisconsin, Rich went to work as a chemist and technology leader for General Electric Company, conducting research for its silicones business. He remained there until he left the company in 2000 to focus on other opportunities – this time with Goodyear Tire in Akron, Ohio.

There Rich ran that firm's global chemistry research before

becoming president of Goodyear Tire's business in North America in 2002.

At GE, Rich had specialized in rubber chemistry, a branch of silicone chemistry that came in handy at Goodyear.

"The skills I had learned as a rubber chemist were applicable in this job," he said. "I also learned about the chemistry side of the tire business."

"The complexity and technology that goes into a tire is amazing."

There were also a few perks with the job. Rich oversaw a rubber plantation in Asia. He also hitched a ride in the Goodyear Blimp several times and even had the iconic symbol fly over his wife's hometown of Jefferson, Iowa.

As president of all Goodyear tire businesses in North America, Rich was also in charge of all the firm's stores, replacement sales, automotive tires and agriculture, mining and aircraft tires.

But his fondness for the silicone industry kept tugging at Rich. So when the

opportunity to become president and chief executive officer of Momentive Performance Materials Inc. became available, which also includes its quartz business, Rich jumped at it. He has been at the Albany, N.Y.-based firm since 2007.

"I've come back to my first love," he says. "I still get to use my scientific background. They just don't let me in the lab anymore."

Momentive is a \$2.5 billion specialty materials firm with 5,000 employees located in 35 countries. It is the second largest producer of silicone-based products and a leading producer of silicon quartz products.

Momentive makes numerous products including bathtub sealants, 2&1 hair conditioners, the rubber pad on your cell phone and Blackberry device, and automotive wiring.

Rich says the importance of silicone products is evident to him everyday.

"I see products that are made by silicone chemistry that people use in their everyday lives," he says. "I like seeing the complicated concepts turn into solutions that effect so many people."

"They may not all be flashy products – although Neil Armstrong's boot used during his historic walk on the moon in 1969 was made out of Momentive's silicone - but that doesn't make them any less important." dg



## Digging in

Iowa State University breaks ground on new chemistry facility

The scoop on chemistry. From left, ISU President Gregory L. Geoffroy; Troy Ross, Carver Trust executive administrator; Bruce Hach; Kathryn Hach; Michael Whiteford, LAS dean; Jake Petrich, chemistry chair; and Dan Saftig, president and CEO of the Iowa State Foundation. Below, Clifford Hach in his lab.

It appeared the groundbreaking ceremony for Hach Hall, Iowa State's newest chemistry building, was going to take place during a cloudy and foggy Saturday morning on Sept. 6.

Minutes before the program was to begin, the sun emerged, brightening the already bright mood of the audience, estimated in excess of 250 people.

Several persons spoke at the ceremonial groundbreaking – construction on the \$74.5 million project had been under way near Gilman Hall for a few weeks. But the star was Kathryn (Kitty) Hach Darrow. The Iowa State alumna and Mukilteo, Wash., resident, was the lead donor to the project with a \$10 million commitment.

Hach Hall is named in honor of Hach Darrow's late husband and ISU alumnus, Clifford Hach, and the extended Hach family. Clifford and Kathryn were longtime

supporters of Iowa State dating back to the 1940s when they met on campus.

"I am thrilled to be part of this transformational opportunity for Iowa State to inspire tomorrow's scientists, teachers, researchers and entrepreneurs," said Hach Darrow. "My husband was a perfect example of someone who saw the potential of science and applied it to improve people's lives. He would be very proud of Iowa State today."

### Chemistry trailblazer

Clifford graduated in 1947 and went on to be a trailblazer and innovator in the chemistry field, and holder of 34 patents. The couple started Hach Chemical Company in 1947 (the name changed to Hach Company in 1980) in Ames and experienced their first major success through

the development of a simplified titration method for measuring hardness in drinking water. Clifford Hach died in 1990. In 1999, the Hach Company became a wholly owned subsidiary of Danaher Corporation.

"Clifford and Kitty never forgot the role that Iowa State University played in their meeting and in the success of the business," said ISU President Gregory L. Geoffroy at the ceremony. "And they have been extremely generous to Iowa State for many years, especially in their support of the chemistry department and scholarships for chemistry students."

Bruce Hach, Clifford and Kathryn's son, told the audience his parents were successful in their business because Clifford, the scientist, worked in the lab while Kathryn handled the business operations.

The groundbreaking ceremony took place near the construction site, at the time a deep hole in the ground south of Pammel Drive in the northwest section of ISU's central campus.

The target finish date for the three-story, 135,000 square-foot facility is June 2010, with occupancy by the Department of Chemistry scheduled for August 2010.

The first floor of the new building will be dedicated to the undergraduate teaching laboratories and student interaction space. The second and third floors will be dedicated to research where faculty, staff and graduate assistants will work. Some labs will be reserved for recruiting new faculty to Iowa State.

The new facility is being built northwest of Gilman Hall, current home to the Department of Chemistry. Gilman Hall will continue to hold general classrooms, computer labs, offices and laboratories.

### Storied history at ISU

"Chemistry has a long and storied history at Iowa State as one of the university's most important and prominent programs," College of Liberal Arts and Sciences dean Michael Whiteford said at the ceremony. "World-class faculty, distinguished graduates and outstanding students are hallmarks of our chemistry program."

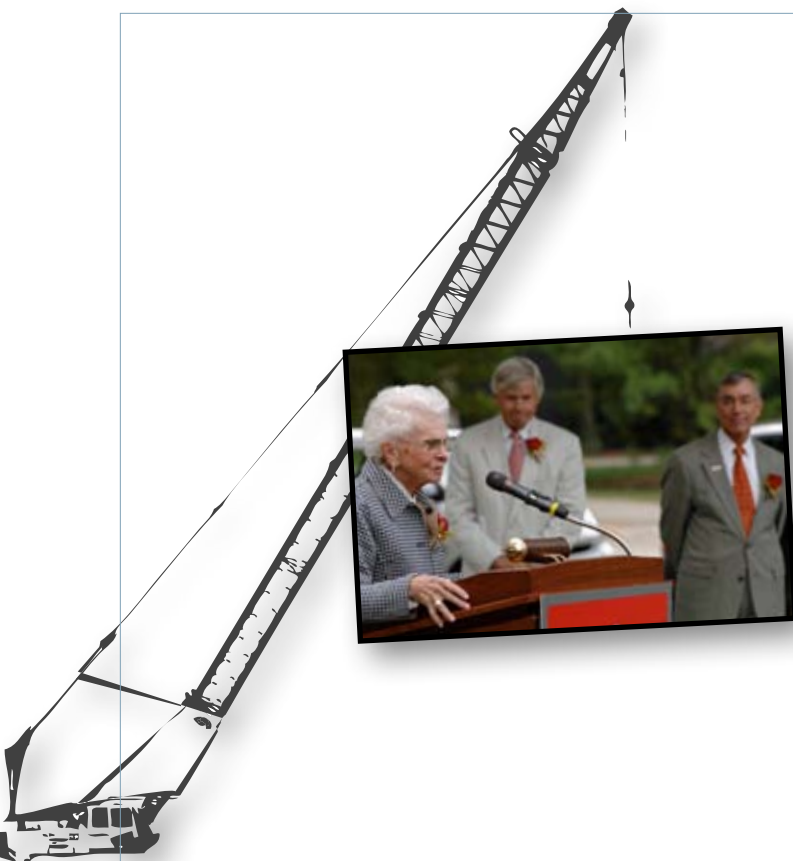
"Now we will have a facility that fits the breadth and depth of the quality of our people."

Jake Petrich, chair of the Department of Chemistry, told the Hach family the department is already benefiting from Hach Darrow's gift.

"We are enjoying the impact of your gift even before the building has been completed," Petrich said. "Thanks to you, we have been able to keep our best faculty at Iowa State, we have been able to attract new faculty and we will have the facilities to continue the best possible research."

Another significant commitment to the project came last year from the Roy J. Carver Trust, based in





Muscatine, Iowa, with a commitment of \$4.5 million to the facility.

### Safe, modern facilities

“The Carver Trust has endorsed this project as a basis for promoting its central interest in biomedically relevant scientific research,” added Troy Ross, executive administrator of the trust. “We recognize the need for providing safe, modern facilities, both for enhancing the existing strengths of the department and as a vehicle for recruiting promising, young investigators to be the chemistry faculty of the future.”

The Iowa Legislature has approved \$58.9 million for the project with an additional \$15.6 million anticipated through private support. Additional private funds raised beyond the \$15.6 million goal will be used for laboratory equipment and classroom enhancements not included in current construction costs.

The commitments from Hach Darrow and the Carver Trust are part of Campaign Iowa State: With Pride and Purpose, the university’s \$800 million fundraising effort that was publicly launched in October 2007.

## Faculty contribute to chemistry building

It’s easy to focus solely on two major gifts in the fundraising campaign for the new \$74.5 million chemistry building project at Iowa State University.

After all, the \$10 commitment from Kathryn (Kitty) Hach-Darrow, Iowa State alumna and Mukilteo, Wash., resident, is the lead gift in the \$15.6 million campaign. Plus the Roy J. Carver Charitable Trust grant of \$4.5 million helped jumpstart the campaign.

But support for the project has been received in numerous quarters including chemistry alumni and even an Iowa State graduate with no connection with the department (see story on page 11).

Those contributing to the project also include a number of current and retired faculty members of the department. One of those contributors is Bob and Jenna McCarley of Ames. Bob McCarley served on the chemistry faculty from 1957 to 1997, including a four-year stint as the department chair between 1973-77.

“Most people don’t appreciate how unique the physics/chemistry/mathematics/metallurgy/chemical engineering connection is here at Iowa State through the Ames Lab,” Bob McCarley said. “The situation is so nice that it made Ames and Iowa State a tremendous place to do chemistry.

“I was extremely lucky to stay on here.”

Because of that deep appreciation for the department, the McCarleys didn’t hesitate to make a contribution to the new Hach Hall.

“I’ve always wanted to give my support to the department,” Bob McCarley said. “I realized we needed a new building to

remain competitive in hiring and retaining the very best faculty members.”

McCarley said he first became concerned about the state of Gilman Hall when he was chair of the department in the ’70s. He said that even then the building was outdated and while the renovations throughout the next couple of decades helped, it didn’t change the need for a new facility.

“I could see the great need for a facility,” he said. “It is essential for the recruitment of faculty and graduate students and even recruitment of undergraduate students.

“Jenna and I recognized the need for a new building and felt we should contribute.”

A new government policy that allows those age 70 and-a-half and older a tax break to make such contributions made it easier for the couple to make a significant contribution.

While the contributions of Hach-Darrow, the Carver Trust, the McCarleys and many others have pushed the chemistry building campaign over the initial goal, efforts to raise more for the facility are continuing.

“When Kitty Hach made her commitment to the campaign, she wanted to be certain her gift would be a motivation for others to give – not a signal that the campaign was successfully completed,” said Alsatia Mellecker, executive director of development for the College of Liberal Arts and Sciences.

“Even though we have reached the original project goal of \$15.6 million, in the spirit of this generous commitment from the Hachs, we continue to work with alumni and friends on additional gifts that will be used for laboratory equipment and classroom enhancements not included in current construction costs.” **dg**

# Giving back

## Gene Lange is not a chemist, but gives support to Hach Hall

Gene Lange’s transcript at Iowa State University shows majors in history, government and modern languages.

Nowhere in that transcript does chemistry even appear.

“I lasted just three weeks in my freshman chemistry class,” says Lange, a 1969 ISU graduate. “Chemistry and I didn’t mix well. It quickly became clear to me I wasn’t prepared to take that class.”

So Lange shifted his interests and moved into the humanities and social sciences at Iowa State.

“I wanted to expand my horizons and it took that chemistry class to make me realize the sciences weren’t for me,” he said.

After graduating, he attended law school at Georgetown University and is now a successful partner with the law firm of Lange, Thomas & McMullen in Washington, D.C.

He is also the owner of Union State Bank in Winterset, Iowa.

So, why in the world, given his lack of interest and association with chemistry over the years, would Gene Lange be featured in a Department of Chemistry alumni newsletter?

Because Lange has contributed \$150,000 to the construction of Hach Hall, Iowa State’s newest chemistry building.

### Change of heart

When Lange and his wife Jeanie arrived on campus in the fall of 2007 for the kickoff celebration for Campaign Iowa State: With Pride and Purpose, the couple was prepared to make a contribution to Iowa State and to one of the College of Liberal Arts and Sciences many academic programs.

Chemistry was nowhere on their radar screen. Lange’s mind was soon changed.

“I attribute my decision to two people,” Lange said, “Burton Christensen and my wife.”

Christensen, a 1952 chemistry graduate and retired senior vice president of Merck Research Lab, was on campus to receive an award from the College of Liberal Arts and Sciences.

After the campaign kickoff ceremony, the Langes went back to their hotel where they ran into Christensen and his wife. The couples sat in



the Gateway lounge and talked about the evening.

“The conversation always drifted back to the chemistry department, and Dr. Christensen made it clear that, while chemistry was an excellent department, it was in need of enhancements, particularly to its facilities, if it was to maintain and improve on that excellence,” Lange said.

“My original leanings were to contribute to one of the social sciences or business departments, but my wife, who isn’t an Iowa Stater, noted that one of the highest priorities on campus and in LAS was the chemistry building. She said it made more sense to put our resources where the most good would come of it,” Lange continued. “Jeanie cleared things up: ‘Why give to any other area when here was this great need and it was a priority of the university.’

“I feel in order to build up the entire university, first you have to build up its finest programs and chemistry is one of those.”

### Giving back

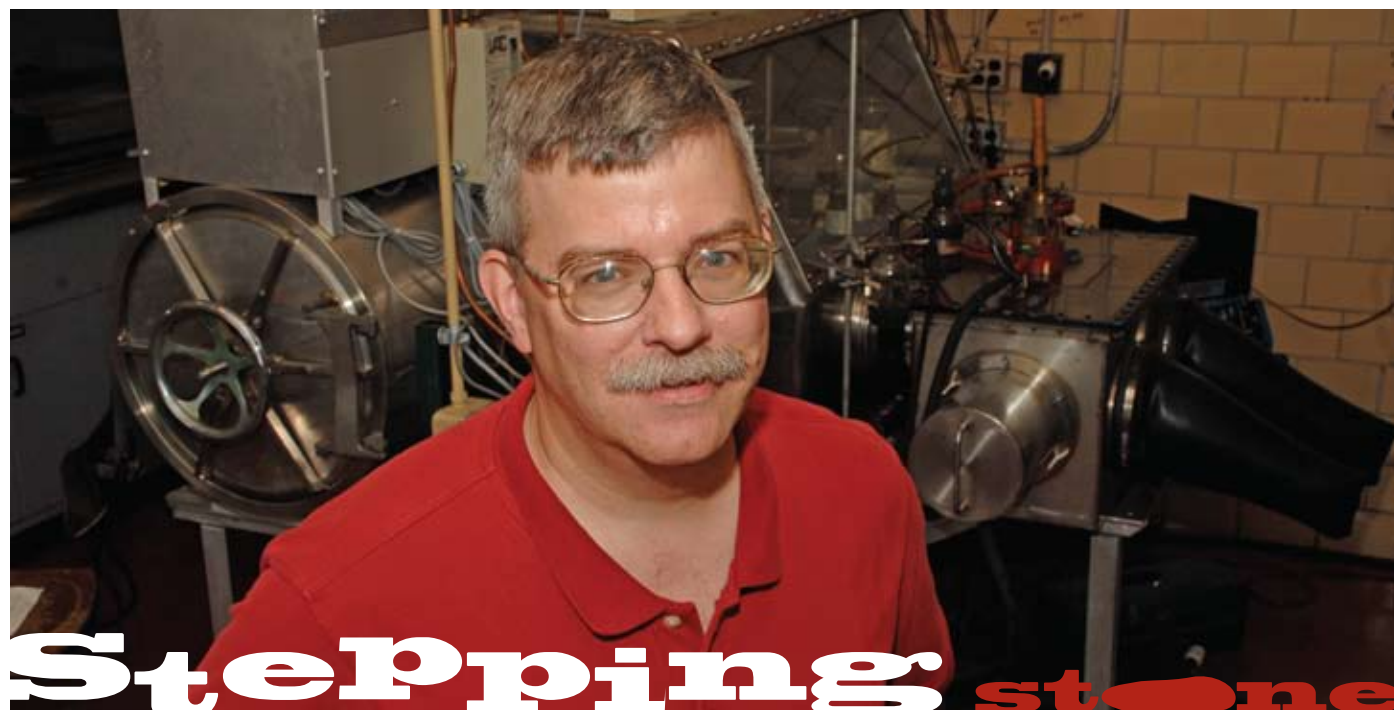
As an undergraduate at Iowa State, Lange was not only involved in several majors but numerous activities as well. He participated in any number of department clubs, was a member of Tau Kappa Epsilon fraternity, served as co-chair of VEISHEA his senior year and was a member of Cardinal Key.

Once he graduated though, he left Iowa State in the rear view mirror and headed to the nation’s capital.

“I spent the first 20 years of my adult life trying to get out of Iowa and the next 20 trying to get back in,” he said. “Iowa State prepared me well for life after graduation. Now I want the opportunity not only to give back to Iowa State financially, but in other ways as well.”

A member of the College of Liberal Arts and Sciences Dean’s Advisory Council, Lange is a frequent visitor to campus these days. He attended the groundbreaking ceremonies for Hach Hall and is excited about the direction of the chemistry department and Iowa State.

“I can’t equate what I have done for the chemistry department with what the Hach family has done,” he said. “But I’m pleased to be able to help somewhat with one of the university’s top priorities.” **dg**



In theory, Gordon Miller's work leads to solid-state results.

When Gordon Miller left his upstate New York farm home for college in the 1970s, many expected his return in a few years as the town doctor. Miller was considering a medical degree during his undergraduate days at the University of Rochester – until he started spending time in an inorganic chemistry research lab.

A professor of chemistry, Miller thought his chemistry courses would be a stepping stone to medical school. But he started making materials in the lab.

“That was a turning point for me,” said Miller. “Inorganic chemistry fascinated me. I found research much more interesting than the prospect of medical school.”

In late 2007 Miller's contributions to the solid-state chemistry field were honored by his being named a fellow by the American Association for the Advancement of Science (AAAS).

Miller was one of five from Iowa State honored in 2007 by AAAS, the world's largest general science organization. The others were Philip Becraft, associate professor of genetics, development and cell biology; Marit Nilsen-Hamilton, professor of biochemistry, biophysics and molecular biology; David Lynch distinguished professor emeritus of physics and astronomy; and Jacob Petrich, professor and chair of chemistry.

Miller's distinction, according to AAAS, honors his work in combining theory with experimentation to study chemical bonding and electronic structure in complex, metal-rich solids.

His group's research efforts combine theoretical investigations with a variety of experimental approaches to “tailor new inorganic materials that will show interesting chemical and physical properties,” he said.

The group is currently researching complex intermetallic compounds to better understand relationships among composition, structure and properties. Aluminum is the primary component of the work.

“We use theory to provide possible interpretations of our experimental results, in particular, to rationalize and even predict the sites for various elements in complex intermetallic structures.”

He says his research team simply wants to answer the question, “Where are the atoms?” Miller said theory is crucial to understand intermetallic compounds because, unlike organic chemistry, this field “doesn't have as many rules guiding the composition of stable compounds.”

Explained Miller, “There are no simple, general models available for describing structure-property relationships in these phases.” His work is aimed at getting enough of an understanding to develop some rules.

The theories Miller's group use have a significant “qualitative” aspect.

“Although we rely on computational work, the level of theory we use can range from simple, theoretical models to complex, exhaustive computations,” he said. “The goal is to provide a picture, or a conceptual understanding, of what the theory says, with the hope of using these ideas in the laboratory.”

Miller entered the field of solid-state chemistry while in graduate school at the University of Chicago. He spent a summer at the renowned Max Planck Institute for Solid State Research in Stuttgart, Germany. He enjoyed it enough that he returned after graduation as a post-doctoral researcher and stayed three and a half years.

“It was an opportunity to work in a foreign country,” Miller said. He learned the language and immersed himself with the German culture.

He returned to the U.S., landing at ISU. It turned out to be a good move because, “Ames, Iowa, is a good location for a solid-state chemist,” Miller said. “Iowa State and the Ames Laboratory have a tremendous reputation in solid-state chemistry.” **sj**

## PIRE initiatives

Theresa Windus aspires to promote NSF international research program.

For someone who was a triple major in mathematics, chemistry and computer science as an undergraduate, Theresa Windus has the “perfect job.”

Windus, a professor of chemistry and an associate with the U.S. Department of Energy's Ames Laboratory, specializes in theoretical quantum chemistry – the science to understand and predict the molecular behavior of matter and energy.

She uses all of her majors as the Iowa State principal investigator for a National Science Foundation project funded through the Partnership in International Research and Education program. The goal of PIRE is to introduce undergraduates, graduate students, post-doc fellows and even some high school students to global research and collaboration with international scientists.

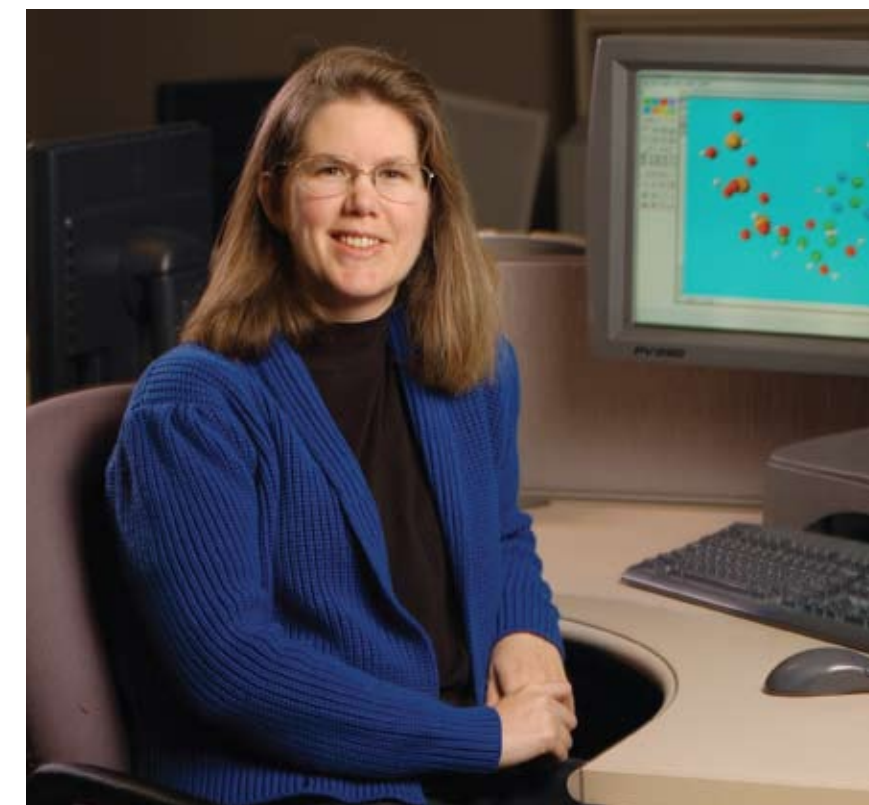
The PIRE project is engaged in several initiatives. Graduate research fellowships, seminars and workshops, study abroad research experiences and collaborative research projects are planned.

“We want to give students an idea that science is worldwide,” explained Windus. She added that the five-year project will provide research experience for students and that members of underrepresented groups will be recruited.

Several PIRE research collaborations between U.S. scientists and international counterparts exist. Windus and ISU are part of a PIRE group that includes Yale and Texas Tech along with university researchers in Austria, Italy and Spain. Her group is using theoretical and computational chemistry to develop and apply algorithms and software to study the interactions of oxygen with organic compounds.

In the interactions, Windus explained, “chemicals will essentially jump to another energetic surface and the products of the reaction are quite different than what we might expect if it didn't make this surface crossing.”

Modeling the reactions is anything but



simple, and Windus' collaborators are building a sophisticated cyber infrastructure to do the simulations. Their infrastructure must interface the diverse and computationally intense work of the researchers.

“It's an extremely difficult chemistry to model,” she said. “It's going to be very challenging, but it will give us the ability to start looking at reactive surfaces that we couldn't have looked at previously.”

The work is basic science, but with some very practical applications, such as protecting space shuttles. When a space shuttle reenters earth's atmosphere, intense temperatures result. The oxygen gets hot and etches the craft's surface.

“We're trying to understand how that etching happens and if there is a way to make materials that etch less,” Windus said.

Windus started college with her eyes on becoming a computer scientist. As a freshman at Minot State University in North Dakota, she took a chemistry course because she needed the science credits.

“I really didn't like it,” she recalled. “They threw a lot of facts at you really fast and didn't tell you why. I like to know why everything works.”

Because of her a high grade in that course, the department chair persuaded her to take another chemistry course. She agreed, basically because she still needed another science course. This time it clicked. “I loved it,” she said.

A Ph.D. in chemistry at ISU and post-doctoral work at Northwestern followed. She held a Department of Defense position then worked several years for the Department of Energy. She was moving up in management, but it wasn't the direction she wanted to go. She came to ISU in 2006 for her first academic appointment.

“I decided I wanted to get back to basic research,” Windus said. “This position just fits me so perfectly because I get to help graduate students, undergraduates and post-docs grow their careers. And I get to do the science that I love to do.”

She recently enjoyed teaching a beginning undergrad chemistry class for 200 non-majors. “It was really fun,” she said. “If I can get even one of those students to love science or even like science, that would be an awesome accomplishment.” **sj**

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