Inside

The Whistle

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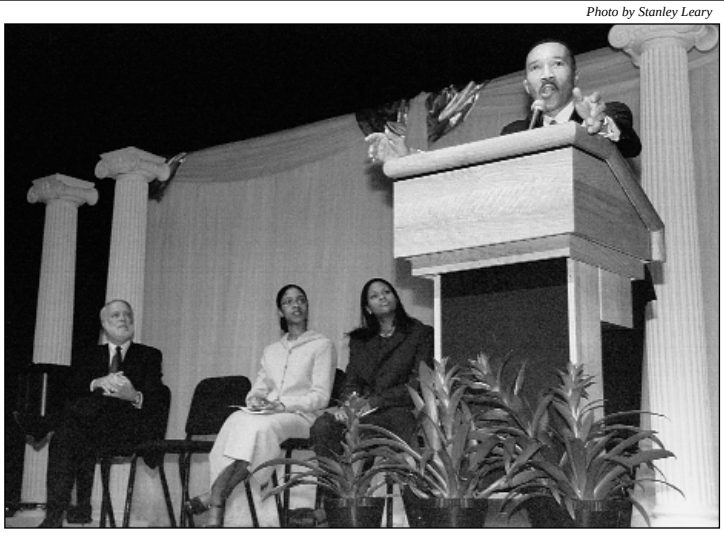
Photo by Stanley Leary



NAACP president challenges FOCUS students with call for social action

Speaking in front of approximately 1,300 students, faculty and other observers in the Robert Ferst Center, NAACP president and CEO Kweisi Mfume charged prospective graduate students to remain vigilant of the inequities — economic, social and educational — that persist in America. "While [education] is not a guarantee of success," he said, "it is a precondition to survival." Mfume also praised President Clough (seated, far left) and Tech for a "demonstrated desire to get young [African-American] men and women focused" on continuing their education. Mfume delivered the keynote address of the four-day FOCUS program.

New supercomputer center helps chemists understand complex reaction processes

John Toon
Research News and Publications

One of the most powerful academic supercomputers in the Southeast forms the core of Georgia Tech's new Center for Computational Molecular Science and Technology. Installed in October, the 72-processor IBM SP supercomputer allows researchers to study complex chemical processes, modeling the hopping of electrical charges and breaking of chemical bonds at a level of detail no other technique could provide.

Though the results must still be verified experimentally, computational chemistry allows scientists to ask more complex questions and get faster, more detailed answers without mixing the first chemical. The technique provides clues to chemical engineering mysteries that cannot be investigated any other way, and reduces trial-and-error in research.

At the new research center, Tech researchers study protein folding and anti-cancer drugs, as well as molecules key to the vision process and the polymerization process.

"If you can do the experiments on the computer and try all the 'what-ifs' that way, at the very end, the one reaction you really need can be done in chemistry," said Rigoberto Hernandez, assistant professor in the School of Chemistry and Biochemistry. "By finding the very best solution on the computer, you can limit the waste products by eliminating trial and error. This doesn't do away with experimentation, but it gives the chemist another tool."

Hernandez studies non-equilibrium reactions in which the

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Marie Curie exhibit underscores importance of women to atomic science

Sean Selman
Institute Communications and Public Affairs

An exhibition that examines the pioneering work of Marie Curie, the discovery of radioactivity and the contributions of women scientists opened Monday in the Neely Gallery of Georgia Tech's Library and Information Center.

In "The Legacy of Marie Curie: One Hundred Years of Science Innovation," patrons learn about the latest discoveries in the areas of medicine, oil and gas exploration, power generation, pharmacology, astronomy, archaeology and geography — all based on studies of the atom.

Among the items featured in this traveling tour will be original laboratory equipment used by Madame Curie in her work, on loan from the Musee Curie in Paris. This exhibit, assembled by curators at Texas A&M University, is the first to display the equipment in the United States. Georgia Tech's Woodruff School of Mechanical Engineering and the Library and Information Center are the primary sponsors of the exhibit's Atlanta visit.

Ward Winer, the Eugene C. Gwaltney Jr. Chair in Manufacturing at Tech and Chair of the Woodruff School of Mechanical Engineering, said it is fitting that the Institute bring the Curie exhibit to Atlanta.

"Tech has several programs that involve the study of radioactive materials, a field in which Madame Curie was an early and prominent contributor," Winer said.

Winer also said it is important for the Institute to highlight the role and contributions of women in nuclear science by hosting this exhibit.

"Although women have not been in science and engineering in large numbers, they have in fact been major contributors to these disciplines for more than 100 years," he said. "Marie Curie and other women featured in this exhibit are among the leaders."

More than 4,100 women were enrolled at Tech in fall 2000 and, of those, more than 60 percent are pursuing degrees in the College of Engineering and the College of Sciences. Also, according to the Engineering Workforce Commission's national statistics on engineering degrees granted between 1993 and 1998, the College of Engineering led the nation in the total number of degrees and the number of undergraduate engineering degrees awarded to women.

The importance of higher

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Preparing the Curie exhibit, from left, are archivist Susan Illis; Gena Poe, a Woodruff School graduate student; records manager Kirk Henderson; and Crit Stewart, assistant director for library access services.

Call for faculty committee nominations

Committees of the faculty have an important responsibility for guiding many of Georgia Tech's activities. With committee elections approaching, the Nominations Committee is seeking interested candidates. Forward your nomination, including self-nominations, by February 5 to Doug Allen, Chair, Nominating Committee, by e-mail (doug.allen@arch.gatech.edu) or campus mail (College of Architecture mail code 0155), indicating for which committee or committees the nominations are designated.

The Nominations Committee will assemble the ballot, and elections will be held during the Spring Semester. The Standing Committees of the General Faculty and of the Academic Faculty are listed at right. For a complete listing of present memberships, minutes of the committees and further details of the election procedures, visit the faculty governance web site at http://www.facultysenate.gatech.edu/. Contact committee chairs or other members to find out more about their activities.

Committees of the General Faculty
(open to all faculty members with general faculty or academic faculty status)

- Faculty Benefits Committee
- Faculty Honors Committee
- Faculty Status and Grievance Committee
- Statutes Committee
- Academic Services Committee
- Welfare and Security Committee

Committees of the Academic Faculty
(open to faculty with academic appointments)

- Undergraduate Curriculum Committee
- Graduate Curriculum Committee
- Student Regulations Committee
- Student Activities and Financial Affairs Committee
- Student Grievance and Appeal Committee.
- Student Honor Committee
- Student Computer Ownership Committee

Open call for nominations designating outstanding women in the Tech community

The Women's Leadership Conference seeks to honor outstanding female individuals from Georgia Tech. It's an opportunity to acknowledge the leadership at Tech provided by many of the women on campus.

Do you know of an undergraduate student, graduate student, faculty member, staff member or an alumna of Tech who deserves some recognition?

Nomination forms are available in the Office of the Dean of Students, Suite 210 of the Student Services Building. Nominations are due Monday, February 5.

Faculty Honors nominations begin

The Institute Faculty Honors Committee is soliciting nominations for awards in the following six categories:

- Distinguished Professor Award
- Class of 1940 W. Roane Beard Outstanding Teacher Award
- Class of 1940 W. Howard Ector Outstanding Teacher Award
- Outstanding Service Award
- Outstanding Continuing Education Award
- Outstanding Interdisciplinary Activities Award
- Outstanding Innovative Use of Education Technology

Descriptions of the awards and nomination requirements may be found at http://www.me.gatech.edu/institute.facultyawards/.

Send nomination packages to:
Jeffrey L. Streator
Room 4206, MRDC I
School of Mechanical Engineering
Georgia Institute of Technology
Atlanta, GA 30332-0405

Campus mail: 0405

All nominations must be received by February 15, 2001. Questions may be addressed to jeffrey.streator@me.gatech.edu or 894-2742.

Georgia Tech

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education to women was not lost on Marie Curie, who in 1867 was born into a family that valued education. As a young woman, she left her native Poland and went to Paris to study mathematics, physics and chemistry at the Sorbonne, where she met and married Pierre Curie. Melding their academic interests, the couple soon established a research relationship.

The Curies' research into radiation earned them the Nobel Prize for physics in 1903, an honor they shared with Henri Bacquerel. Eight years later, Madame Curie received a second Nobel Prize, this time in chemistry, for her discovery of polonium and radium and for research that isolated radium and studied its chemical properties. Curie was the first person to receive the Nobel Prize twice and remains the only woman so honored.

The importance of Madame Curie's initial discoveries regarding radioactivity deserves the recognition offered by this exhibit. Her findings changed society's view of the subatomic world. Today, more than a century after Curie's work began, radiation permeates daily life and has a vast range of scientific and practical applications — from the frequent use of X-rays to cutting-edge discussions of particle physics.

Among the other Nobel Prize-winning women featured in the Curie exhibit are her daughter, Irene Joliot-Curie, who earned the prize for chemistry in 1935; Maria Goeppert Mayer, who garnered the prize for physics in 1963; Dorothy Crowfoot Hodgkin, who was awarded the prize for chemistry in 1964; and Rosalyn Sussman Yalow, who received the prize for medicine in 1977.

Other prominent scientists profiled in the exhibit are Lise Meitner, a physicist who offered the first theory on nuclear fission; Rosalind Franklin, whose X-ray photographs of DNA led to the discovery of its double-helix shape; and Florence Rena Sabin, who conducted pioneering research on blood, bone marrow and tuberculosis.

"This exhibit offers a wonderful chance for the Woodruff School to sponsor something that is of more general interest for the campus, our alumni and the Atlanta community," said Rona Ginsberg, director of communications for the Woodruff School of Mechanical Engineering. "We are eager for the public to attend, perhaps people who might not normally visit Tech. They will see a wonderful exhibit that highlights women in science, and perhaps have a chance to view some of our facilities and see the campus."

The free exhibit runs through March 2 and is open to the public. Its hours are 10 a.m. to 4 p.m. daily. Extended viewing hours will be offered Wednesdays until 8 p.m. and 10 a.m. to 2 p.m. Saturdays. For more information, call 894-4529 or refer to **www.me.gatech.edu/me/curie/**

Chemistry, continued from page 1

reacting chemicals form a large part of the overall environment. In common chemical processes, the reactants make up a small part of the overall environment, which remains in equilibrium, not changing substantially as the reaction proceeds.

But in non-equilibrium systems, the environment changes as the reaction proceeds, affecting the chemistry in ways that are difficult to model and study. This complex interaction between reaction and changing environment affects the outcome in important ways.

"In many cases, the final properties of the material are determined by their history," he explained. "I want to understand how things are formed, not just to characterize their properties once they are formed."

Protein folding provides an important example. After being created, proteins fold through a complex chemical process that involves as many as 200 different amino acid residues. Different folds give the proteins different properties. In some cases, such as amyloidogenic proteins associated with Mad Cow Disease, a wrong fold creates a harmful protein: the scrapie form of prions.

"There is increasing evidence that the wrong folds are due to a kinetic or dynamic process," Hernandez added. "We as dynamicists are asking how a sequence with a given structure goes to that folded structure. By understanding those dynamics, we would be able to say something about altering the sequence and preventing it from folding that way."

David Sherrill, an assistant professor in the School of Chemistry and Biochemistry and Hernandez's collaborator at the center, studies electronic structure theory and its application to photochemistry and highly reactive systems. His work has implications for improving anti-cancer drugs, understanding the process of vision and tracing the role of copper in the body.

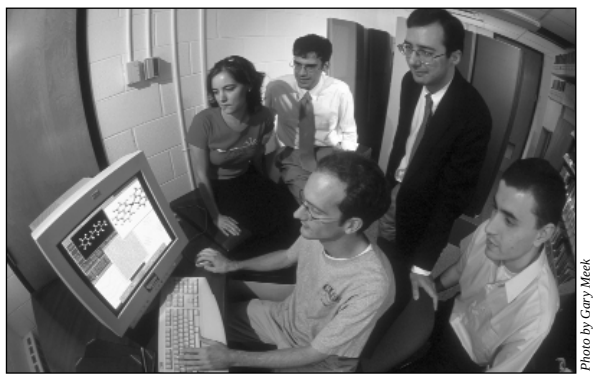

Photo by Gary Meek

Practicing 'chemistry without chemicals': From left, Rebecca Locker, Rigoberto Hernandez, Marc Vogt, David Sherrill, and Mutasem Sinnokrot.

The enediyne family of anti-cancer drugs provides a vital weapon in the battle against the dread disease. The highly reactive chemicals contain two radicals that steal hydrogen atoms from the DNA of cancer cells, triggering destruction of the cells.

Although experiments have shown the basic steps of the diradical reaction, detailed computer models could give new insights into how to tune the reactivity by adjusting the chemical structures of the drugs. Having that information would help scientists produce better anti-cancer drugs.

These computational studies will require the development of new theoretical techniques because current models can't accurately describe the highly reactive diradicals, or more generally, any bond-making or bond-breaking processes.

"To get a very detailed understanding of the whole process, going from reactants to products and watching it happen in-between, you usually are breaking chemical bonds," Sherrill explained. "You would like to be able to describe that theoretically, including the entire reaction path, not just the beginning and the end."

The IBM SP supercomputer installed at the center in October promises a dramatic increase in the speed at which simulations run, doing in a few hours what would have taken a week of number-crunching on smaller computer workstations. It also allows researchers to undertake more complex and accurate simulations that they could not even attempt before.

"This will allow us to do some very high accuracy calculations on some benchmark molecules that were inaccessible before," said Sherrill. "It will make a tremendous difference."

Because the reactions Hernandez and Sherrill study are so complex, limits on computing power have forced them to rely on approximations that do not take into account all the variables that could influence the outcome. The supercomputer will alter that trade-off, enabling simulations with fewer compromises.

By speeding up the simulations, the machine will also change the way in which the researchers work, allowing them to be more productive and creative in following up unexpected results.

"If you have a calculation that takes a week for you to complete, you've got to have a lot of different things going on at once while you're waiting for the calculations to be done," Sherrill explained. "But if you could get the results in a couple of hours, you could immediately see what didn't work and how to change it. You could be a lot more interactive, and recover more quickly from mistakes."

Based on IBM's new copper chip technology, the machine will be shared with other researchers at the College of Sciences.

Seeking to shore up low blood reserves, the local chapter of the American Red Cross has called upon the Tech community to assist. The blood drive, sponsored by the American Red Cross, the MOVE Office, and the Co-op Club, January 23 to 25, from 10 a.m. to 4 p.m. in the Student Center Ballroom. For more information, contact 894-2002 or move@programs.stucen.gatech.edu

Working in a traditional Japanese method, North Carolina-based artist Susan Olsen presents her latest series of work, "Images from Nature," as the first installment of 2001 in the Robert C. Williams American Museum of Papermaking, located in the Institute of Paper Science and Technology.

It was during her visits to Japan that she learned the technique Obara Washi, the form she experiments with today, in which processed and unprocessed fibers are juxtaposed within each sheet of handmade paper in order to portray landscapes and other natural imagery. Such pieces accentuate the hues of the natural fibers she uses in her paintings, giving them a more organic, lifelike quality. Creating her pulp paintings from their origins in nature, Olsen plants, cultivates and harvests her own plants before processing the fibers for papermaking, which becomes the canvas for another of her process-oriented works.

On display through March 23, the museum is open during the week from 9 a.m. to 5 p.m. For more information, contact the museum at 894-6663, or refer to www.ipst.edu/amp.

Susan Olsen, "January Day," pulp painting, 2000