Quantum Computing: 
*Leaping Forward*

Computers are getting faster and smaller, with more and more hardware compressed onto smaller chips. Gordon Moore (B.S. 1950, Chemistry), co-founder of Intel, correctly predicted 26 years ago that the number of transistors per semiconductor chip would double every 18-24 months.

Indeed, within the next two decades, experts believe that transistors, devices that regulate the flow of electricity in electronics, will be on the atomic scale. And at the atomic level, particles and systems no longer behave in well-understood classical ways. Instead quantum mechanics, the theory that elementary particles have wavelike properties, takes over.

Classical computers operate according to classical physics, where particles have defined positions and motions. “Most people forget that computers work by performing operations on fundamental units called bits,” said Ken Brown, a researcher in Professor Birgitta Whaley’s group.

A bit resides in a specific memory location, stores either a 1 or a 0, and is manipulated by logic gates, which transform bit values in defined ways, such as changing a 1 to a 0. A 1 may contain 10,000 electrons and a 0 may have only 10 electrons. Since the differential between a 1 and a 0 is quite substantial, these two states can be distinguished.

However, as electrical storage devices shrink to atomic scales, it will become impossible to distinguish between the two states. At the quantum level, a system that can be in one of two states is technically not in either state before it is measured, nor is it in any other state! Confusing, but in quantum systems, particles are no longer well-defined, but are described by waveforms and have specific probabilities of being in a specific state at a specific time; however, there is no way to know which state before measuring the system.

“In quantum computing the bits are replaced with qubits,” said Brown. Qubits are fundamental quantum logic units that, according to quantum mechanics, can be both 1 and 0 at the same time! Since the individual logic units in the computer now involve, simultaneously, both 0 and 1, operations on these qubits can produce more

Schaffer and Yang Awarded NSF CAREER Grants

David Schaffer, Assistant Professor of Chemical Engineering, and Peidong Yang, Assistant Professor of Chemistry, have each received a prestigious 2001 CAREER Award from the National Science Foundation. The highly competitive five-year grant provides a total of $375,000 of support. Schaffer does research on improving the viral gene delivery vehicles used in gene therapy, and Yang devises new ways to make nanowires and nanotubes.

“I was happily surprised to win this award. I didn’t expect to get it on my first try,” Schaffer said.
IBM Awards College a Grant of Supercomputing Equipment

Theoretical chemistry at Berkeley is getting a welcome boost in computing power. Chemistry Professor Martin Head-Gordon, and colleagues David Chandler, William Miller, and Birgitta Whaley in the Pitzer Center for Theoretical Chemistry, have received a very generous equipment grant from IBM to upgrade the IBM SP2 (scalable parallel) computer in the facility.

According to Head-Gordon, this computer will assist in enabling parallel algorithm development within the theory groups. “Modern theoretical chemistry is closely tied to high-performance computing, so state-of-the-art resources are essential,” said Head-Gordon.

The grant is part of the IBM “Shared University Research” (SUR) program, which is available to Berkeley and competitor institutions. “We are very happy to see the College get its second SUR grant in three years,” noted Head-Gordon. The first grant brought the basic SP2 machine to the Pitzer Center a few years ago.

According to Dr. Jean Paul Jacob, manager of the external technical program for IBM Almaden Research Center, the upgrade to the SP2 machine will allow the theoretical chemistry group to tackle computational problems of scale to obtain new insights into a variety of chemical questions.

College Hosts Successful Mini-Statistical Mechanics Meeting

The College of Chemistry hosted a mini-Statistical Mechanics meeting in January, with Professor David Chandler presiding. Over 80 attendees spent a day and a half listening to 15 lectures and an evening viewing nearly thirty contributed presentations, all of which provided a healthy sampling of the latest research in the field.

According to Chandler, the meeting was an unqualified success. “The invited presentations were uniformly excellent, stimulating much interest and discussion. Of all the interesting ideas put forth, the three talks that seemed to create the most excitement were those by George Oster, Professor of Cell and Developmental Biology at Berkeley, on the workings of ATPase; by Hao Li, from UCSF, on a pattern recognition algorithm applied to decoding the genome; and by Peter Wolynes, from U.C. San Diego, on the theory of glass formation,” Chandler observed.

Professor Chandler himself has been in the news recently. In an article in the March 16 issue of Science, his research group studied the fundamental details of water ionization and discovered the source of water’s ability to ionize weak acids and bases. Ions may disperse readily in water, which itself autoionizes into H3O+ and OH- ions. Using a combination of molecular dynamics calculations and a method for efficient sampling of water’s potential energy surface, Chandler’s group found that water ionization combines fluctuations in the long-range electrostatic interactions with hydrogen-bond dynamics. Ions produced usually recombine quickly, but when the fluctuation coincides with the breaking of the hydrogen-bond wire, the system crosses a transition state and the ions cannot recombine quickly.

“Additionally, IBM has a certain interest in the group’s findings,” Dr. Jacob said. “IBM has the Blue Gene project that aims at gaining insight into protein folding and some of the computations done by the Berkeley professors will help. Some of the most innovative molecular dynamics is performed by these professors, and IBM is proud to support their work.”
Communicating Chemistry:  
*Turning the Tables on Students*

Loud conversation filled the room as 40 elementary school children sat at tables topped by large tubs of water. Cal students filed through the door, filling out nametags in big bold letters. Today was the first time in Communicating Chemistry, Physics and Astronomy 100 they would try out their training with eager, attentive pupils, all 2nd through 4th graders at Hillcrest Elementary School. The undergraduates had been preparing for this for the past few weeks under the direction of Professor Angelica Stacy, one of the course instructors.

The class began with an activity designed to help everyone get to know one another: the children became “tape recorders” as the Cal students talked about what they knew about science back when they were in elementary school themselves. They then “rewound” the children and had the “recorders” repeat back what they heard, to the delight of the kids.

Next, the Cal students spread out among the tables. There were different stations set up for “floating,” “sifting,” and “magnetism,” and the college students had prepared questions for the youngsters to help teach scientific principles, such as why wax floats on water but steel sinks, and why lima beans stay trapped in the colander, whereas sand sifts through.

“We have two objectives in this course,” said Dr. Stacy. “First, we want the Cal students to become better communicators and anticipate the needs of the person receiving the information. It’s very difficult sometimes to explain scientific concepts on an elementary level once you’re in college; you forget what it’s like to be that age. And second, we are performing a service to the community. We take nationally tested materials and experiments and introduce them to the teachers as well as the children in their classes. Some teachers from years past have repeated these experiments on their own. It’s a good trade: the science majors at Cal get exposure to the teachers and the teachers learn from the Cal students.”

According to James Rice, a senior in chemistry, the class has taught him two important principles. “We have learned both how to relate to kids and how the learning process takes place. It’s nice because we guide the kids to the explanation of a scientific principle without telling them the answers to our questions straight out.”

And the elementary students got a kick out of the learning stations. “It was a lot of fun,” said fourth-grader Sam Sugarman.

“Communicating Chemistry:  
*Turning the Tables on Students*”

Students from Hillcrest Elementary get a hands-on science lesson from Cal undergraduates.

“We don’t usually do these things in class. We got to get our hands dirty.”

The Cal students will travel to local elementary schools throughout the semester, in groups of two or three, and teach science experiments for a total of six hours. They will receive one unit of course credit, according to Professor Stacy.

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**Outreach to Silicon Valley**

In its second foray into Silicon Valley, the College of Chemistry is teaming up with the College of Engineering to present “Berkeley in Silicon Valley: New Directions in Chemistry and Engineering,” on Saturday, June 9. This faculty and networking forum will feature a keynote address by Dr. Stephen Fodor (Postdoc, 1990), president and CEO of Affymetrix, followed by faculty presentations of the cutting-edge research that makes the Colleges of Chemistry and Engineering among the most distinguished in the country. The presentations will focus on three topics: bio-MEMs, biomaterials, and the miniaturization of electronics. For more information, see the College of Chemistry website: www.cchem.berkeley.edu, or contact Camille Olufson at (510) 643-7379 or at colufson@cchem.berkeley.edu.
complex results than operations on classical bits. And, if a large number of qubit logic units are coherently connected together in a single quantum state, then a single quantum mechanical operation on that system can be equivalent to a very large number of operations on classical bits.

Quantum computing may sound like science fiction—computers powered by calculations on waveforms rather than on individual bits—but it is becoming closer to reality, thanks to work by imaginative scientists, including some here at Berkeley.

Chemistry Professor Birgitta Whaley and her colleagues are working on ways to protect quantum systems from decoherence. Decoherence occurs when a quantum system interacts with its environment and loses its quantum character, becoming a classical system in the process. Manipulating the qubits can destroy the coherent superposition of the system and cause it to revert back to classical bits.

“The field right now is very interdisciplinary,” remarked Professor Whaley. “We work with computer scientists who do the encoding, as well as physicists and mathematicians. Chemists are just starting to venture into this field now because quantum computing has moved beyond theoretical calculations into becoming a reality. And in the real world, nothing is isolated, all systems interact with other systems.”

Theoretical scientists have already found algorithms that can be used for large-scale quantum computers, but one has yet to be built with more than 5–7 bits. Scientists have built a 7-qubit computer using NMR, since NMR can be used to manipulate and measure nuclear spins, which serve as qubits. However, NMR quantum computers are intrinsically limited because the signal-to-noise ratio is so low. So researchers are motivated to look for other systems that can serve as the basis for quantum computers.

There are different approaches: one popular system is a gas-phase system that can be totally isolated so decoherence does not occur. Another is one that weakly interacts with its environment, such as quantum dots or a condensed-phase system. This is most likely going to be what allows scientists to build large-scale quantum computers.

“However, decoherence will occur when the quantum state interacts with an outside environment,” Whaley explained. Decoherence can occur not only when a system is manipulated and measured, but when it interacts in any way with the outside world, such as a slight vibration or a stray photon. “My group is working on several possible solutions, one of which is encoding and error correction. If we assume from the beginning that errors due to decoherence will occur, then we can account for them and correct for them when we set up the system.”

Scientists are still debating the uses of quantum computers. Quantum computers will very likely be used for encryption programs, which use the factoring of large numbers to restrict access to certain files and locations. Classical computers take a very long time to factor large numbers since they operate on their bits one at a time, but quantum computers could do similar calculations with qubits in a matter of minutes. Quantum computers will also find a home in modeling quantum chemistry problems, since many of the variables in quantum mechanics are too complicated for classical computers.

And many of the applications for quantum computers are not yet even known, according to David Bacon, a researcher in Whaley’s group. “As recently as the 1970s, no one had a clue that classical computers would be everywhere, from desktops and laptops, to chips in your toaster and microwave. I think the uses for quantum computers will become known as the field advances.”
“It gives me a lot of flexibility in developing both my research group and a new lecture and lab course curriculum for bioengineering.” Schaffer is also the recipient of an Office of Naval Research Young Investigator Award for the year 2001 to “analyze the regulation of adult neural stem cell behavior.”

Schaffer and his group work with directed evolution, sequentially generating random mutations in proteins and analyzing them for specific properties, to increase the applicability of gene therapy. Over the past decade, directed evolution has become one of the most efficient ways to engineer new functions into proteins.

Gene therapy, the insertion of a therapeutically beneficial gene into a patient’s cells to cure disease, is very promising. Last spring, researchers in France announced the apparent cure of two children who lacked a gene critical in producing a working immune system. However, there are still technical challenges to overcome.

“One of the specific problems with gene therapy that I am interested in overcoming is that of in vivo gene expression shutdown—that is, once the therapeutic gene is integrated into the target cell’s DNA, it slowly becomes recognized as foreign. The gene gets turned off, and the protein encoded by that gene is no longer expressed in those cells,” Schaffer explained. “By altering the gene sequence, we can hopefully eliminate this gene silencing and allow the therapeutic genes to be properly expressed.”

Schaffer is also developing labs and lectures for the undergraduate bioengineering course to reflect changes in the biotechnology industry. “We are adding new lecture material focusing on recombinant DNA and directed evolution,” Schaffer said. In parallel, a new graduate course is in the works on bioinformatics and gene diversity (to be offered in 2003) that will host speakers from different departments.

Peidong Yang, in addition to the NSF CAREER award, has been named an Alfred P. Sloan Research Fellow. The Sloan Foundation grant of $40,000 is designed “to stimulate fundamental research by young scholars of outstanding promise.”

Yang’s research focuses on nanoscience—specifically on nanoscale chemistry in one dimension. A nanometer is one-billionth of a meter; the diameter of the hair on your head is about 250,000 nanometers. Nanoscience encompasses a wide range of issues, since at such a small scale, quantum effects come into play and manipulating the individual components of nanosystems is increasingly complicated.

Yang and his group are creating the building blocks for future nanodevices. “We are approaching this issue from three angles. The first is to discover new chemistry to make nanowire building blocks, the second is to utilize these nanowires to form complex nanostructures and understand their properties, and the third is to build and understand functional nanodevices in different systems,” he said.

“Nanotechnology has made tremendous progress in the last few years. A lot of the chemistry has been worked out, and we are starting to understand how to rationally synthesize the nanowires and nanotubes. We are now focusing on how to assemble these pieces and give them specific desirable properties, such as light-emitting diodes, field-effect transistors and nanolasers,” Yang continued.

According to Yang, one of the most promising applications of nanotechnology is its use in the information storage and computer industry. “For example, we are making tiny UV/blue nanolasers that operate at room temperature. We expect at least a four-fold increase in data density when they replace conventional gallium arsenide red lasers. This means more data and movies can be packed onto a single compact disc.”

“And Berkeley has really been a fantastic place to do research,” Yang remarked. “This university has great facilities on campus and attracts talented graduate students who contribute a lot to my research. We really enjoy doing research here.”
Paul Alivisatos, Professor of Chemistry, was recently named editor of the new journal *Nanoletters*, published by the ACS.

Nitash Balsara, Professor of Chemical Engineering, has been named a Fellow of the American Physical Society.

Kristie Boering, Assistant Professor of Chemistry, has been named a recipient of a Hellman Family Faculty Fund 2000 Award.

Alex Pines, Professor of Chemistry, received the Dickson Prize from Carnegie-Mellon University. He will also deliver the Jacob Bigeleisen Lecture at Stony Brook, the Laird Lecture at the University of British Columbia and the Inaugural Regitze Vold Memorial Lecture at University of California, San Diego. He has also been named an Alan S. Tetelman Fellow of Yale University.

Gabor Somorjai, Professor of Chemistry, has been awarded an honorary Doctor of Science degree from the University of Manchester.

Andrew Streitwieser, Emeritus Professor of Chemistry, has been awarded a Camille and Henry Dreyfus Foundation Senior Scientist Mentor Initiative for 2001 to support undergraduate research workers.

Dirk Trauner, Assistant Professor of Chemistry, has been awarded a Camille and Henry Dreyfus Foundation Senior Scientist Mentor Initiative for 2001 to support undergraduate research workers.

## ACS Award Winners to be Honored in April

The American Chemical Society (ACS) is honoring two College of Chemistry faculty members. Chemistry Professor Carolyn Bertozzi will be awarded the *ACS Award in Pure Chemistry*, sponsored by Alpha Chi Sigma Fraternity. Chemical Engineering Professor Alexis T. Bell will receive the *ACS Award for Creative Research in Homogeneous or Heterogeneous Catalysis*, sponsored by Shell Oil Foundation. The awards will be presented to these two outstanding scholars in April at the 221st ACS national meeting in San Diego.

Professors Carolyn Bertozzi and Alexis Bell will be recognized at the spring ACS meeting.