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Newsletter

HAROLD JOHNSTON WINS TYLER PRIZE FOR ECOLOGY-ENERGY WORK

MMRD Faculty Senior Scientist HAROLD S. JOHNSTON, Professor of Chemistry at UCB, has been named a co-winner of the Tyler Prize, the largest ecology-energy prize in the world. Johnston shares a cash award of $150,000 with F. Sherwood Rowland of UC Irvine and Mario. J. Molina of U.C. Irvine and the Jet Propulsion Laboratory.

The award recipients are being honored for "their scientific breakthroughs in atmospheric chemistry and their farsighted efforts to prevent the depletion of the earth's ozone layer." Gold medals were presented at an awards ceremony in Beverly Hills on Wednesday, May 25.

Johnston, one of the world's leading authorities in the field of atmospheric chemistry, first drew

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REYNOLDS, LESTER DEVISE CHEMICAL PROPERTY CALCULATION METHOD

Ground-state energies for molecules that are gratifyingly close to the experimental values have been calculated using the quantum Monte Carlo method devised by PETER REYNOLDS, MMRD Staff Scientist, and WILLIAM A. LESTER Jr., UCB Professor of Chemistry and MMRD Faculty Senior Scientist.

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NATIONAL ACADEMY OF SCIENCES ELECTS FALICOV, JEFFRIES, THOMAS

Four LBL researchers, including three MMRD Faculty Senior Scientists--LEO FALICOV, CARSON JEFFRIES and GARETH THOMAS-- were elected members of the National Academy of Sciences at its annual meeting held in Washington, D.C. late in April. Falicov and Jeffries are Professors of Physics and Falicov is also chairman of the UCB Physics Department. Thomas is Professor of Metallurgy at UCB and is Scientific Director of MMRD's National Center for Electron Microscopy (NCEM).

The fourth LBL scientist elected is GEORGE TRILLING of the Physics, Computer Science, and Mathematics Division; he is also a Professor of Physics at UCB.

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SCHAEFER WINNER OF ACS LEO BAEKELAND AWARD

MMRD Faculty Senior Scientist HENRY F. SCHAEFER III, UCB Professor of Chemistry, has been named winner of the 1983 Leo Hendrick Baekeland Award, one of the most prestigious presented by the American Chemical Society (ACS). It is given biennially to a chemist under 40 years of age and consists of a gold medal and an honorarium.

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NATIONAL ACADEMY OF SCIENCES
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Falicov is regarded as a leading theorist in the study of condensed matter; his work on the electronic properties of solids has led to new understandings of the optical and magnetic properties of solids, and of the surface properties of alloys, metals, and semiconductors.

Jeffries is a leading experimentalist studying crystal structures and electrical properties of solids. He was the first to photograph and analyze electrons in the form of a liquid droplet inside a supercooled crystal wafer. His current highly innovative experiments are demonstrating how order breaks down into chaos in nonlinear systems, a key physical phenomenon.

Thomas has achieved a long list of "firsts," recognized by the highest honors in electron microscopy and metallurgy. His pioneering work with increasingly powerful microscopes has resulted in the establishment of the NCEM at LBL, which now includes the 1 MeV Atomic Resolution Microscopy (ARM), as well as the year-old 1.5 MeV High Voltage Electron Microscope (HVEM), and a number of other high-resolution instruments.

Trilling is a leading experimentalist in properties of nuclear particles and a key member of the Berkeley-Stanford team using the Stanford Linear Accelerator, discovering entire new families and properties of particles of matter, including the psi family and charmed mesons.

HAROLD JOHNSTON WINS
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general attention to the possibility that stratospheric contamination might threaten the earth's ozone layer. In a 1971 paper in Science, he proposed that nitrogen oxides could reduce ozones in the earth's upper atmosphere. He further suggested that globally significant amounts of nitrogen oxides could be directly injected by a proposed fleet of high-altitude supersonic aircraft. In 1974, he won the Pollution Control Award of the American Chemical Society.

"In the last decade," stated the announcement made by the University of Southern California, administrators of the John and Alice Tyler Ecology Fund, "he has applied progressively more sophisticated laboratory methods in the search for greater understanding of the interactions of nitrogen oxides and other gas molecules in the atmosphere. During this brief period, the research in this field has progressed from a primitive state to advanced satellite monitoring of nitrogen oxides in the upper atmosphere."

The Tyler Prize was established in 1973 by Mrs. Alice C. Tyler and John C. Tyler, a founder of the Farmers Insurance Group. The prize is awarded for achievements related to ecology, environmental conditions, and the development of energy sources. A Tyler Award Reception in honor of Harold was held June 3 in the LBL cafeteria.

JEFFRIES AND SOMORJAI ELECTED TO ACADEMY OF ARTS AND SCIENCES

CARSON D. JEFFRIES and GABOR A. SOMORJAI, MMRD Faculty Senior Scientists, have been named fellows of the American Academy of Arts and Sciences. Jeffries was one of four new members elected to the Physics section; Somorjai and one other scientist were honored for work in chemistry. Both MMRD investigators are UCB professors.

Seventy-seven fellows were elected to the Academy from throughout the country.

Founded in 1779 by John Adams, the Academy is devoted to the cultivation and promotion of all branches of the arts and sciences. It is located in Boston.

TOBIAS ELECTED TO NATIONAL ACADEMY OF ENGINEERING

CHARLES W. TOBIAS, UCB Professor of Chemical Engineering and Faculty Senior Scientist in MMRD, has been elected to membership in the National Academy of Engineering. Election to the Academy is the "highest professional distinction that can be conferred on an engineer and honors those who have made important contributions to engineering theory and practice or who have demonstrated unusual accomplishments in new and developing fields of technology." Tobias was cited for being an outstanding pioneer and leader in developing electrochemical engineering into a quantitative discipline based on fundamental principles.

Tobias was one of 49 engineers selected this year from the United States, bringing the total Academy membership to 1142, with 102 foreign associates.

GRONSKY WINS BURTON MEDAL

RONALD GRONSKY, MMRD Staff Scientist and manager of the Atomic Resolution Microscope Facility in the National Center for Electron Microscopy at LBL/MMRD, will be awarded the 1983 Burton Medal. Confered by the Electron Microscopy Society of America (EMSA), the award is given annually to recognize outstanding research contributions in electron microscopy by a young investigator.

Gronsky has made significant contributions to the study of interfacial defects in metals, alloys, and semiconductors.

The award will be presented at the EMSA annual meeting, to be held in Phoenix this summer.

SCHAEFER WINNER OF ACS
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Schaefer is being recognized for his "exceptional achievements in the application of electronic structure theory to chemistry . . . . The more theoretical thrust of his research has been directed at one of the most challenging problems in molecular quantum mechanics, the problem of electron correlation in molecules," the ACS said in announcing the award. His work has also "guided experimentalists into new and fruitful directions."

The award is sponsored by Union Carbide Corporation to commemorate the technical and industrial achievements of Leo Baekeland, who invented the first commercial plastic 75 years ago and founded the General Bakelite Company, which Union Carbide later purchased.

Presentation will be this fall by the North Jersey Section of the ACS. Schaefer will be honored at a dinner to be hald in Washington, D.C., during the ACS national meeting and at an award dinner and symposium to be held in New Jersey.

The Baekeland Award was first conferred in 1945. The present one is the first in 30 years for a Berkeley chemist, the previous winner being MMRD Faculty Senior Scientist LEO BREWER, UCB Professor of Chemistry.

REYNOLDS, LESTER DEVISE
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Physicist Reynolds says he is hopeful about further improving the accuracy and eventually extending

the approach to calculate other chemical properties as well. The method uses a Monte Carlo random-sampling technique to solve the Schrödinger wave equation for the molecules under study. It requires a large computer, preferably a supercomputer, and much mathematical ingenuity.

The Schrödinger wave equation describes the behavior of quantum mechanical entities such as the electron, protons, and neutrons that make up a molecule. Because each of these entities behaves in a way that depends on all the others, solving the Schrödinger equation poses an enormous theoretical challenge.

The Monte Carlo technique itself was developed several decades ago, primarily for use in nuclear and solid state physics, and only recently has it been applied to chemistry. Monte Carlo is useful for mathematically describing events that are random in nature, such as diffusion and radioactive decay. However, it also can be used to calculate integrals and to solve equations. The trick is to make the equations "look like" random processes.

To solve the Schrödinger equation with Monte Carlo methods, the equation is reshaped into two parts, one resembling the equation for diffusion and one resembling that for radioactive decay. Then the Monte Carlo method simulates the entire Schrödinger equation as a combination of these two statistical processes.

Quantum Monte Carlo can give an exact solution in principle, but in practice two kinds of error are present and must be dealt with--statistical and systematic. Statistical error can be reduced by increasing the amount of computer time used and by using a technique called importance sampling (sampling most where the wave function is largest). The second, systematic error, is small; however, the researchers are currently investigating a number of ways to reduce it still further.

So far, Reynolds and Lester, partly in collaboration with scientists at Lawrence Livermore National Laboratory, have calculated molecular energies for five simple molecules having from 2 to 10 electrons. Their results are more accurate than those given by other approximation methods, and even better accuracy seems achievable. Reynolds says that quantum Monte Carlo may have wide application in chemistry because of its relative ease of computation and its potential for high accuracy.

MMRD SCIENTISTS RECEIVE AIME AWARDS AT MEETING

LEO BREWER, Faculty Senior Scientist, SUBRAMANIAN SURESH, former MMRD Postdoctoral Research Associate, and JAMES W. EVANS, Associate Faculty Scientist, were honored at the 112th annual meeting of the American Institute of Mining, Metallurgical, and Petroleum Engineers (AIME), held in March in Atlanta.

Brewer, a UCB Professor of Chemistry, was awarded the 1983 William Hume-Rothery Award, which has been presented annually since 1972 by the Metallurgical Society of AIME "to honor an outstanding scientific leader, in recognition of his scholarly contributions to the science of alloys." He also opened the Hume-Rothery Memorial Symposium on Phase Stability and Thermodynamic Modeling, giving a talk on "The Role of Electronic Configuration in Determining Structure and Stability."

Dr. Suresh, a lecturer in UC Berkeley's Department of Materials Science and Mineral Engineering,

received the Robert Lansing Hardy Gold Medal in recognition of "outstanding promise in the field of metallurgy by a metallurgist under the age of 30 (as reported in the March Newsletter).

Evans, a professor in the UCB Department of Materials Science and Mineral Engineering, was recipient of the 1983 Extractive Metallurgy Science Award, given for a paper entitled, "A Mathematical Model for Prediction of Currents, Magnetic Fields, Melt Velocities, Melt Topography, and Current Efficiency in Hall-Heroult Cells." Co-authors were Yury Zundelevich, Bechtel, and Devraj Sharma, Dames and Moore.

MMRD SCIENTISTS STUDY PATTERNS OF CHAOS IN PHYSICAL SYSTEMS

CARSON D. JEFFRIES, UCB Professor of Physics and MMRD Faculty Senior Scientist, has reported experimental confirmation of the presence of certain universal patterns along the "period-doubling route to chaos," in an April UC Berkeley Physics Department Colloquium. His talk, "Deterministic Chaotic Dynamics," described his study of chaos, defined as "the erratic behavior of systems completely determined by equations of motion." Development of erratic noise in semiconductor systems as the driving voltage is increased is an example.

Scientists studying new phenomenon find that chaos in physical systems has proved not to be as erratic as it appears. Rather, certain universal patterns occur as systems are driven harder, until the onset of some kind of noisy instability. In other words, the route to chaos may be predictable if the system is deterministic.

Professor Jeffries, working with graduate students Jose Perez, James Testa, Gloenn Held, Paul Bryant, and George Gibson, has been conducting experiments on solid-state systems that exhibit chaotic behavior. "This work was triggered by intriguing theoretical developments of the past few years in nonlinear dynamics," said Jeffries. "These theories have been developed by mathematicians and theoretical physicists the world over, including some very important work here at Berkeley."

Jeffries' work has experimentally confirmed the "period doubling route to chaos." That is, the time in which the driven current in semiconductor or magnetic devices repeats itself is progressively doubled: 2,4,8,16, etc. Chaos begins at the point when the period has doubled so much that it has become infinite. After the inception of chaotic behavior, a pattern of periodic windows ensues--islands in a sea of chaos.

It is interesting that this complicated dynamical structure can be "semiquantitatively understood by an extremely simple equation (called the logistic map) given to us by nonlinear dynamics theorists," said Jeffries. "This simplification can be understood in terms of the new theoretical framework which proposes that chaotic behavior exhibits some kind of universality. That is, there are some recognized patterns of behavior well defined quantitatively by universal numbers.

NEIL BARTLETT AWARDED NICHOLS MEDAL BY N.Y. CHAPTER, ACS

Professor of Chemistry NEIL BARTLETT was awarded the William H. Nichols Medal by the New York chapter of the American Chemical Society in March. A Faculty Senior Scientist in MMRD, he is the latest in a line of Berkeley researchers who have been given what is said to be the oldest ACS award (see March Newsletter).

"It was nice to receive a medal that has gone to so many prestigious people," says Bartlett. He was recognized primarily for his synthesis work, including the first compound of a noble gas. The award, established in 1903, has been presented to six other Berkeley Professors of Chemistry: Gilbert Lewis, Joel Hildebrand, Glenn Seaborg, Wendell Stanley, Wendell Latimer, and Melvin Calvin. Other recipients include Linus Pauling, Peter Debye, and Roald Hoffmann.

"I'm sure that the award committee recognized that we were still managing to do decent work," Bartlett comments with typical British understatement. He is especially excited about the graphite research which his group has been working on over the last five years.

"The research we've done has indeed been good and helped clarify some important issues in graphite chemistry," he says. "In fact, (graduate student) Tom Mallouk has found a way of making highly fluorinated graphite at room temperature. He has shown that you can take graphite, fluorinate it, and reduce it electrochemically. Meanwhile, the graphite maintains its flat-sheet structure. That's rather nice.

"It's a new kind of bonding of carbon to fluorine," he explains. "It is semi-ionic, and involves one-electron bond covalency. This contributes to the important property that you can make and unmake this material electrochemically."

His group has done a variety of synthesis work, discovering the +5 oxidative state of gold, creating the first salts of the perfluorobenzene cation (the first "metallic" salt of layer-form BN), and synthesizing a range of oxidized graphite compounds.

Bartlett's group is presently interested in what electrical behavior may be found in creating graphite/BN alloys.

MMRD RESEARCHERS ON "MOST CITED SCIENTISTS" LIST

LBL Director and Professor of Chemistry DAVID A. SHIRLEY and UCB Professor of Physics MARVIN L. COHEN are among the top 300 on the list of "1,000 Contemporary Scientists Most Cited." Both are Faculty Senior Scientists in MMRD.

Also on the list are EARL C. MUETTERTIES and HENRY F. SCHAEFER III. Both are UCB Professors of Chemistry. Muetterties is Associated Faculty Scientist and Schaefer is Faculty Senior Scientist at MMRD.

This issue of the list was published in Current Contents, October 12, 1981, by the Institute of Scientific Information and covers the period 1965 through 1978.

CLARKE WINS "DISTINGUISHED TEACHER"

JOHN CLARKE, Professor of Physics at UCB and Faculty Senior Scientist in solid state physics at MMRD, is one of seven UC Berkeley professors named April 26th as the campus' distinguished teachers for 1983. He was noted by students for his sense of humor, his high regard for students and, as one student wrote, the fact that "he also erases the blackboard more thoroughly than anyone else I know"--an important factor in a physics class. The awards include cash and certificates, given by the Academic Senate and the California Alumni Association and presented at a campus ceremony.

NEW HONOR FOR GLENN SEABORG

LBL Associate Director GLENN SEABORG, Professor of Chemistry at UCB and MMRD Faculty Senior Scien-

tist, received his 49th honorary degree, Doctor of Science conferred by the University of Pennsylvania on March 11.

During a recent trip to the East Coast, Seaborg attended the International Convocation for World Environmental Regeneration in New York. He also gave a speech, "A Preview of the National Commission on Excellence in Education," to the Universities Research Association Council of Presidents; additionally, he presented a paper on "Nuclear Reactions and Synthesis of New Transuranium Species" at the National Academy of Sciences.

HEINEMANN AUSTRALIAN LECTURES

HEINZ HEINEMANN, MMRD Staff Senior Scientist and Lecturer in Chemical Engineering at UCB, presented a lecture course in Petroleum Catalysis for the Australian Petroleum Institute at the University of Melbourne in mid-April. He also gave talks in Melbourne before the Royal Australian Chemical Institute, the Commonwealth Scientific and Industrial Research Organization, and The Australian Institute of Chemical Engineers.

While in Melbourne, Dr. Heinemann was asked to make a stop in Sydney to conduct a seminar in the Chemical Engineering Department of the University of New South Wales. He then also was persuaded to give a lecture at Macquaire University, New South Wales, before embarking on his return trip to Berkeley which featured an R&R stop in Tahiti, with Mrs. Heinemann, who had accompanied him on the entire trip.

FIGHT FOR ANOTHER'S THEORY LEADS TO PRESTIGIOUS AWARD

Sometimes an outsider is needed to champion another's cause. Professor LEO BREWER received the Hume-Rothery Award last month (see MMRD SCIENTISTS, page 4) because he fought for someone else's theory.

The Metallurgical Society of AIME (The American Institute of Mining, Metallurgical, and Petroleum Engineers) presented the award in recognition of what is now called the Engel-Brewer Theory.

The story began during the early '40s when Brewer was working on the Manhattan Project. His research team was trying to create a container for casting molten plutonium, a metal little understood at the time. "I figured that, at its worst, it couldn't be contained," he says. However, the team developed a successful containing compound, CeS, with NaCl crystal structure but metallic appearance. They named it "invincium" and used it to contain many molten metals.

"We melted platinum in a CeS crucible," he recalls. "We were astonished when it chewed up the crucible."

This reaction remained a puzzle until Neils Engel visited Berkeley in 1948 and presented his extension of the Hume-Rothery relationship between crystal structure and electron concentration in transition metals. His model explained the Ce/Pt interaction, but had been rejected by the scientific community. "He sent a manuscript to a physics journal, which rejected it as too empirical," recalls Brewer. "Then he sent it to a metallurgical journal, which rejected it as too theoretical."

Brewer presented the theory to his classes. In the '60s, two of his chemistry 106 students studied the reaction of Pt with ZrC and ZrO_2. The presence of Pt reduced the activity of zirconium metal by a factor of 10^{20} at 1200°C. This and other experiments supported the theory.

Though Brewer's research was in high temperature gaseous

spectroscopy, not metals, he spoke of Engel's idea at symposia. The theory was gradually accepted. Most of its predictions are now confirmed.

"I'm glad to see that Engel's theories are getting recognition and I am glad that I was able to call attention to them," says Brewer.

GARETH THOMAS, MMRD Faculty Senior Scientist and Scientific Director of MMRD's National Center for Electron Microscopy, gave the plenary lecture at the Annual Japan Society for Ceramics Conference, May 17 in Tokyo. His subject was, "Electron Microscopy and Microanalysis In Ceramics." Thomas, a Professor of Metallurgy at UCB, also lectured at NKK Steel, Toshiba, and at Seoul University, Korea.

MMRD PEOPLE

ANTHONY G. EVANS, Professor of Materials Science and Mineral Engineering at UCB, and Associate Faculty Scientist in MMRD, is co-editor of Fracture Mechanics of Ceramics, Vols. 5 and 6, Plenum Publishing Corporation.

KENNETH GAUGLER, MMRD Staff Scientist, has had a letter from the Electron Microscopy Society of America's Education Committee reporting that they have had a steady demand for the "Tuning Your SEM for Optimum Performance" tutorial videotape prepared and produced by Ken last year. As of mid-March, ten universities and two companies had used the tape and there was a waiting list for the three available copies.

DR. PATRICIA THIEL has joined Professor PAUL L. RICHARDS' group as a Visiting Postdoctoral Research Associate. Pat received her PhD at California Institute of Technology and did her initial postdoctoral work at University of Munich's Physical Chemistry Institute. She also worked at Sandia-Livermore.

COLLEEN BORIS will start work in the MMRD Purchasing Office with SANDY STEWART this month.

CARLIE BERKE has joined the MMRD Personnel Office, replacing INGEMAR (MAR) GOSIENGFIAO, who has left to take a job in his field as an architect with a firm in Redwood City.

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