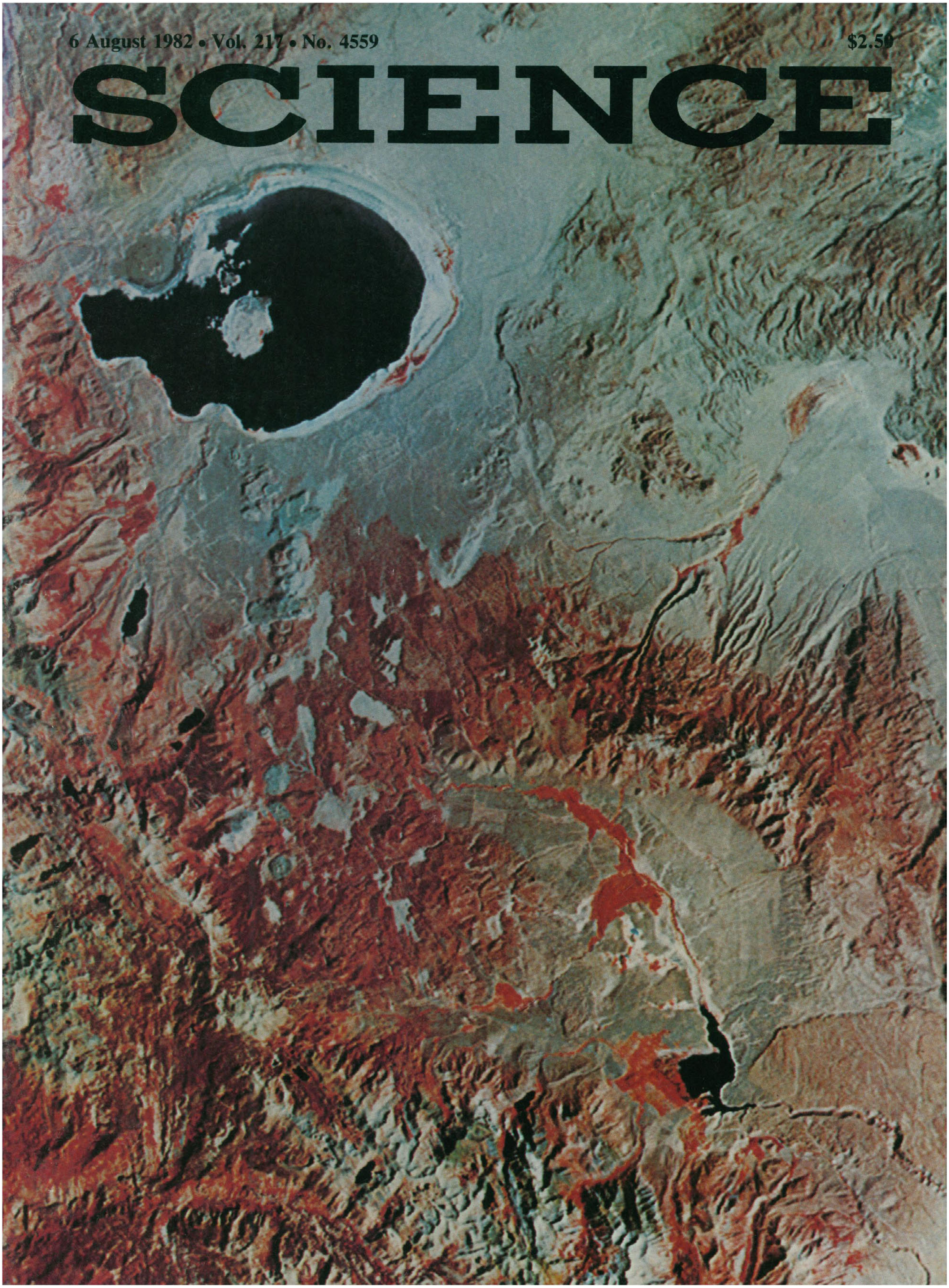
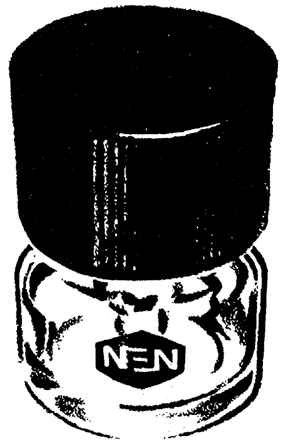
6 August 1982 • Vol. 217 • No. 4559

$2.50

SCIENCE





The secret life of L-Fucose

In the beginning, L-Fucose was in our catalog as a ^{14}C-labeled compound — one of the basics of biological research. People ordered it when they needed it. While new products got all the publicity, L-Fucose was just there.

But at NEN not even old standbys are taken for granted. So, quietly, L-Fucose began a program of self-improvement.

First it was tritiated to give researchers a choice of label. Then, as our chemists developed new methods of synthesis, a version was offered at ten times the previous specific activity. The next step was to add aqueous solution packaging to your options. Most recently we further increased its specific activity to the highest available.

Today L-Fucose is offered in seven forms to meet the varying needs of research.

The point of the story is this: Over 1100 other NEN labeled compounds are undergoing the same scrutiny. So look closely in our catalog before you order. You may well find that the old standby is as up-to-date as compounds making the headlines.

The NEN extras are the biggest bargain in labeled chemicals

NEN New England Nuclear®
a Du Pont company

ISSN 0036-8075
6 August 1982
Volume 217, No. 4559

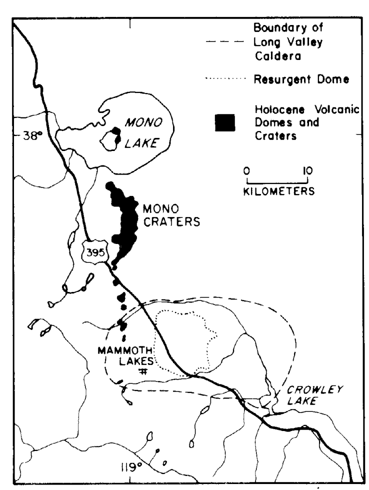
SCIENCE

SCIENCE is published weekly on Friday, except the last week in December, by the American Association for the Advancement of Science, 1515 Massachusetts Avenue, NW, Washington, D.C. 20005. Second-class postage (publication No. 484460) paid at Washington, D.C., and at an additional entry. Now combined with **The Science Monthly**® Domestic individual membership and subscription (51 issues): $48. Domestic institutional subscription (51 issues): $85. Foreign postage extra: Canada $24, other (surface mail) $27, air-surface via Amsterdam $55. First class, airmail, school-year, and student rates on request. Single copies $2.50 ($3 by mail); back issues $3 ($3.50 by mail); classroom rates on request. **Change of address:** allow 6 weeks, giving old and new addresses and seven-digit account number. **Postmaster:** Send Form 3579 to *Science*, 1515 Massachusetts Avenue, NW, Washington, D.C. 20005. *Science* is indexed in the *Reader's Guide to Periodical Literature* and in several specialized indexes.

AMERICAN ASSOCIATION FOR THE ADVANCEMENT OF SCIENCE

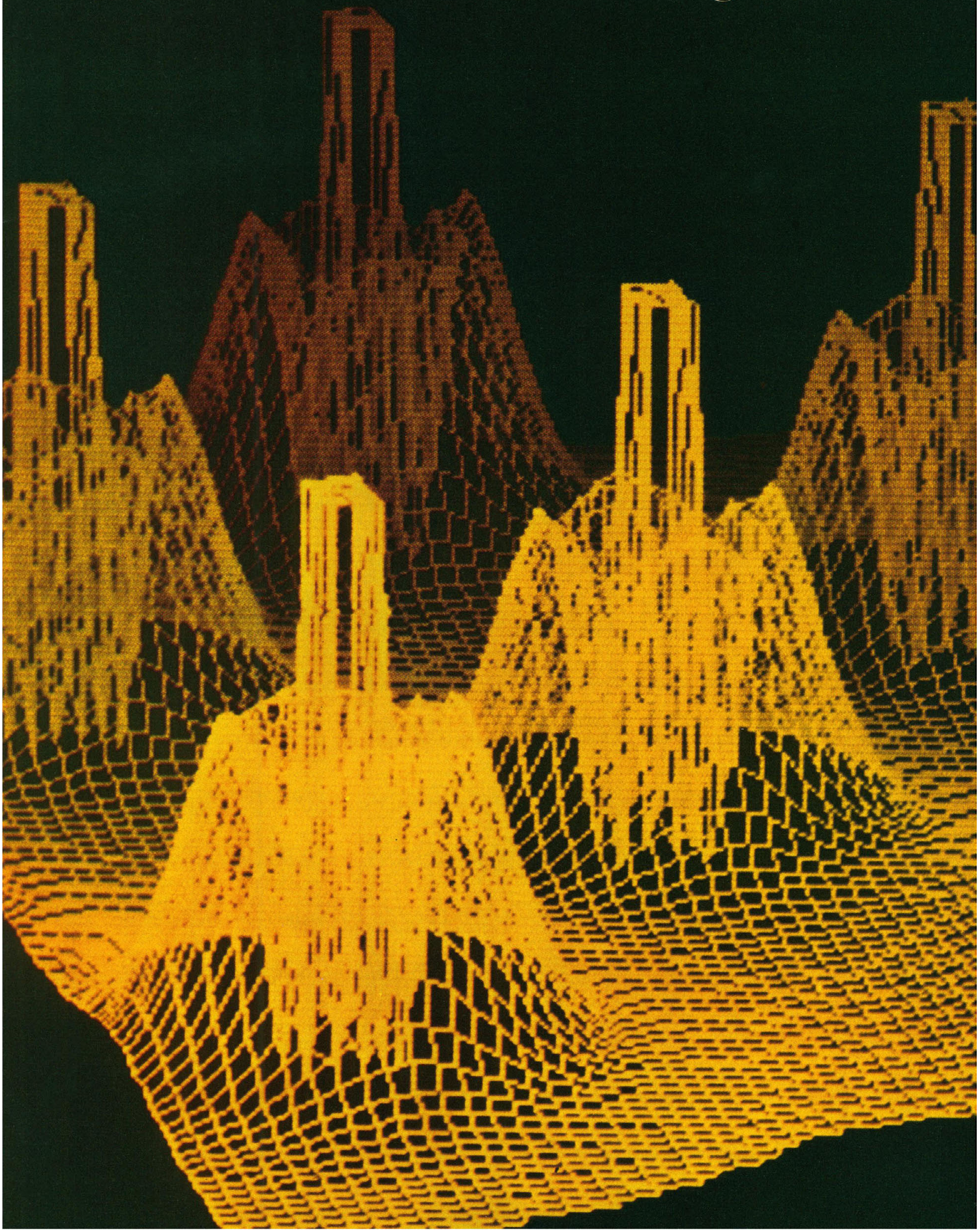
COVER

Area of Quaternary volcanism and faulting near Mammoth Lakes, California. See page 531.



NASA Landsat E-2 951-17300 457 false color, 30 August 1977

The Surface Contingent



The Surface Contingent

A recent finding at the General Motors Research Laboratories has changed scientific thinking about the behavior of electrons in metal surfaces. This discovery provides a greater understanding of the fundamental physical processes involved in such surface events as adhesion, corrosion and catalysis.

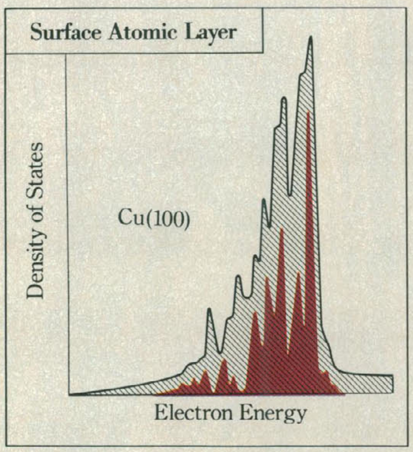


Figure 1: Energy distribution of electrons in outermost atomic layer. Red area indicates electrons in surface states.

Figure 2: Two electron density contour maps of the cross-section of a Cu(100) surface. One map shows a clean copper surface (tan); the other shows a nitrogen-covered copper surface (green).

CONVENTIONAL scientific thought treats virtually all of the valence electrons found in the surface atomic layer of a metal as if they are free to roam throughout the metal's interior. The work of three physicists at the General Motors Research Laboratories suggests otherwise. Through calculations confirmed by experimental data, the theorists have shown that more than a quarter of the valence electrons in the top atomic layer of some metals are effectively trapped in the surface. The presence of so many "surface state" electrons must be considered when analyzing physical and chemical surface phenomena, including such surface events as oxidation leading to corrosion.

Drs. John Smith, Jack Gay and Frank Arlinghaus applied their theoretical analysis to the (100) surface of five metals: copper, nickel, silver, rhodium and palladium. They made bold predictions concerning the percentage of electrons in the surface atomic layer to be found in surface states: Cu(36%), Ni(23%), Ag(23%), Rh(23%) and Pd(19%). The ratio of the red area to the hatched area of figure 1 gives the percentage for copper.

Electrons in surface states are not only abundant, but also highly localized on the surface. Chemisorption on a metal is also confined to the surface region. Figure 2 shows what happens in the case of nitrogen chemisorbed on copper. The two contour maps coincide except in the surface layer, where the interaction is largely exhibited. Localization of the interaction holds for the chemisorption of other gases, including oxygen in the initial stage of metal oxidation. These observations led the physicists to conclude that surface states are important in chemisorption.

One way to probe electrons in surfaces is to chemisorb atoms on a clean metal surface and look for changes in photoemission spectra. Such an experiment was performed at GM for fractional monolayers of nitrogen, oxygen and sulfur on Cu(100). The dominant change in the photoemission spectrum was the disappearance of a large peak whose shape and energy location was independent of the chemisorbed atom. It was of special interest that the shape and energy location of this peak was nearly identical to the envelope around the surface state peaks in figure 1. This suggests that surface state electrons play a major role in the chemisorption process.

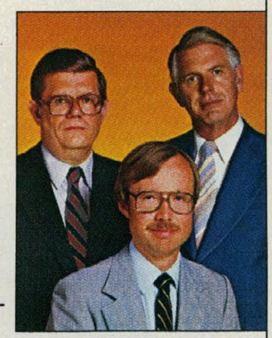
THE THEORETICAL advance at the heart of the discovery is the "Self-Consistent Local Orbital (SCLO) Method" for solving the Schrödinger equation. This new mathematical method was devised by the GM theorists to handle the classic dilemma posed by the self-consistency requirement. The characterization of electron behavior used to complete the equation must be consistent with the behavior predicted by the equation. In other words, one almost needs to know the answer in order to make the calculation.

Self-consistent solution of the equation for a metal surface is made exceedingly difficult by the three-dimensional nature of the electron density distribution. The theorists dealt with this challenge successfully by dividing the electron density distribution into two parts—the first part due to overlapping atomic density distributions; the second part equaling the difference between this atomic contribution and the exact density distribution.

One of the more stringent tests of the accuracy of the SCLO method was an angular photoemission experiment conducted by Heimann et al. at the University of Munich, subsequent to publication of the GM research. The German research team confirmed a prominent surface state band predicted by the three GM physicists. This was the first time a surface state band on a solid had been calculated prior to its being seen experimentally. The SCLO method makes possible something that could not be done before—accurate prediction of the actual behavior of electrons whirling around nuclei at the surface of a metal.

"The large body of surface states we found on metal surfaces," says Dr. Smith, "may be a controlling factor in many physical and chemical surface phenomena. By replacing conjecture with calculation, the new surface theoretical methods give us the means to make major steps forward in the analysis of surface and interface properties."

THE MEN BEHIND THE WORK



Drs. Smith, Gay and Arlinghaus are theorists in the Physics Department at the General Motors Research Laboratories.

John Smith (center) and Jack Gay (right) received doctorates in physics; Smith from Ohio State University and Gay from the University of Florida. Frank Arlinghaus received his Ph.D. in physical chemistry from the Massachusetts Institute of Technology.

John Smith, leader of the GM solid state physics group, did postdoctoral work at the University of California in La Jolla. He joined General Motors in 1972. Frank Arlinghaus and Jack Gay joined the corporation in 1964 and 1965, respectively.

Each member of the team brings to the project a different expertise: Smith in surface physics, Gay in solid state theory, and Arlinghaus in bulk band structure calculations.

SCIENCE/SCOPE

More than 4,500 men and women have furthered their professional careers through the Hughes Fellowship Programs since 1949. Those who qualify are given the opportunity to earn advanced degrees in scientific and engineering disciplines. Under full-study programs, employees study at selected schools and work at a company facility during the summer. Under work-study programs, employees work part-time and carry about one-half of a full academic load at nearby schools. More than 100 fellowships are awarded annually.

The millimeter-wave seeker for the Wasp air-to-ground missile, the first ever to find and track military targets all by itself, achieves its breakthrough by using advanced subminiature hardware and innovative application of the data it gathers. Wasp is intended to let a pilot release swarms of missiles in the general direction of a known enemy force without having ever actually seen it. Special data-processing techniques allow each missile to autonomously detect and hit a separate target, thus making the most of the swarm's effectiveness. Hughes is building eight flight test missiles for the U.S. Air Force.

A new infrared radiation source has been developed at Hughes using a standard polysilicon gate MOS process. The thermal IR source is intended for use inside a dewar without optical windows for testing monolithic focal plane arrays at temperatures as low as 4°K. It illuminates at wavelengths from 4 to 6 millimeters with pulse rise and fall times of 1 microsecond. The source is a tiny, heavily-doped silicon resistor isolated from a thermally sunk silicon substrate by 400 nanometers of silicon dioxide. The resistor can be heated electrically to 50°K with about 100 milliwatts of power. A sapphire filter absorbs wavelengths longer than 6 micrometers; the source is not hot enough to produce many photons with wavelengths shorter than 4 micrometers.

Computer-aided manufacturing is improving productivity in the electronics business, sometimes by as much as a factor of 10 or more. Computers help do production planning efficiently by retrieving proven techniques and testing new situations through simulation. By controlling fabrication, process, and assembly operations, computers assure that each operation will be done right the first time. Such control also permits small runs to be handled with efficiency approaching that of a single-setup run. Hughes is spending $240 million over five years on computer-aided manufacturing. This capital investment is part of a $1.5 billion program for expansion and modernization to improve productivity.

"Diversification" characterizes Hughes Industrial Electronics Group, located in the Southern California communities of Carlsbad, Irvine, Newport Beach, Sylmar, and Torrance. Our facilities are like small companies with 500 to 2,000 employees, but each offers the resources and benefits of a $2 billion company. Our diverse technologies include silicon and GaAs semiconductor technologies, fiber optics, microwave and millimeter-wave communications, microprocessors, lasers, and solar cells. Send resume to B.E. Price, Hughes Industrial Electronics Group, Dept. SE, P.O. Box 2999, Torrance, CA 90509. Equal opportunity employer.

Creating a new world with electronics

HUGHES

HUGHES AIRCRAFT COMPANY
CULVER CITY, CALIFORNIA 90230

(213) 670-1515 EXTENSION 5964

6 August 1982, Volume 217, Number 4559

SCIENCE

Long-Term Changes in the Chemical Industry

A combination of factors has caused the chemical industry to examine its future feedstock and energy sources. At present, petroleum and natural gas are by far the predominant sources of organic carbon and energy. However, increases in the price of oil and natural gas have had impacts on conservation, process design, and choice of future feedstocks. The price of these hydrocarbons will likely tend to rise faster than inflation, creating additional pressure for changes in the industry and in its needs for trained people.

One alternative is coal. As a source of heat, its cost is about one-fifth that of oil or natural gas, and increasingly it is replacing other fuels. Coal can also serve as a source of such compounds as benzene, toluene, phenol, and naphthalene. In future, coal is likely to be consumed in large quantities to make synthesis gas, that is, carbon monoxide plus hydrogen, which can be converted to methanol, ethanol, and a host of hydrocarbons.

But for the long-term future and to meet worldwide needs, the most interesting feedstock is derived from photosynthesis. In contrast to fossil fuels, biomass is renewable, and supplies will likely increase substantially in the coming years. As feedstocks, wood and plant materials are more versatile than coal, and advances in biotechnology are likely to lead to innovative processes for manufacturing chemicals from them.

In terms of ash or sulfur content, plant material is cleaner than coal, and it is converted to synthesis gas more readily. But the really interesting chemicals produced by plants and trees are the diverse natural products, such as rubber, resins, terpenes, carbohydrates (including starch, hemicellulose, and cellulose), proteins, fats, waxes, and lignin. Up to the present, research to improve plants has largely focused on food crops. This effort has been quite successful and indicates that similar efforts would improve the yields of other desired products. Already better management of silviculture in some instances has led to yields five times those of natural stands.

Of all the products of photosynthesis, glucose and its polymers are probably the most important as chemical feedstocks. Glucose is a favorite source of energy and carbon for many microorganisms, both aerobes and anaerobes. They can convert the sugar into hundreds of different chemicals, including ethanol, citric acid, and pharmaceuticals. By use of selected mutants and of recombinant DNA techniques, it should be possible to target specific products and improve their yields.

In spite of the increasing costs of oil and natural gas, the transition to other feedstocks will occur only gradually. The petrochemical complexes are in place. Biotechnology is likely to have its initial expansion in the production of substances that cannot be derived from fossil fuels. But fermentation is beginning to have a small but significant impact on the petroleum industry. Until recently, nearly all industrial alcohol was derived from ethylene. Now an increasing fraction is coming from grain, and some of it is being used in gasoline in an application other than gasohol. Some oxygenated organic compounds, including ethanol, increase the octane number of gasoline and thus serve as a substitute for tetraethyl lead.

For decades, biotechnology was overshadowed by the petrochemical industry. Fermenters producing ethanol, acetone, and butanol were dismantled. The pharmaceutical and food industries kept industrial microbiology alive, but academic training in biotechnology was almost nonexistent. Thus there are few academic experts in the field at a time of expanding opportunity. Some of the nation's most creative people are scientists versed in molecular biology, including recombinant DNA techniques. However, if their work is to lead to the production of useful products for society, biotechnology and biochemical engineers must be involved.

Many of the major chemical companies recognize that important future opportunities involve biotechnology and they are building their staffs accordingly. Students who have inclinations and aptitudes for the natural sciences can confidently seek training in biotechnology with the conviction that the field will expand in significance and usefulness for many decades.

—PHILIP H. ABELSON