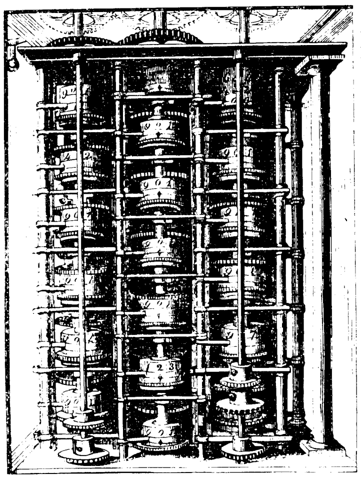
The Incredible Shrinking Computer

The ultimate computer may be one whose miniaturized electronic elements are molecules that can even assemble themselves

By IVARS PETERSON



It would be like having a second brain — a computer small enough to fit snugly in the lining of a helmet but powerful enough to sift through a steady stream of incoming data. Like a preamplifier that prepares a raw musical signal for the more exacting refinements of an amplifier, a helmet-embedded computer could run through tedious data-sorting chores while saving more creative work for its human counterpart.

Visions of such futuristic devices brought more than 150 researchers to the 2nd International Workshop on "Molecular" Electronic Devices, held recently at the Naval Research Laboratory (NRL) in Washington, D.C. Many participants were drawn by the possibility that this meeting would someday, perhaps 30 years in the future, be known as the "birthplace" of the molecular computer. It was a chance to speculate at the very edges of current research. And for some companies, it was a chance to test the waters for commercial possibilities and to stake out claims in uncharted fields.

"The prospect of making computer circuits smaller and smaller is inviting," says Forrest L. Carter, NRL chemist and workshop organizer. The ultimate goal is to synthesize and organize a teaspoonful of molecules into a sophisticated, powerful computer.

Carter says tiny molecular computers would make possible small, intelligent robots. Others suggest medical applications, including devices that bring sight to the blind or, when implanted in the brain, monitor body functions and the brain's electrical system. A naval official foresees computerized helmets that enable pilots to cope with the growing flood of digital data coming from flight instruments and sensors.

Molecular computers already exist — as the brains of living creatures. For some workshop participants, the message was clear: if nature can do it, why can't we? "We know the ideas work because we are here, we move, we sometimes think ...," says Carter. The challenges involved in building a digital molecular computer, however, are awesome.

In essence, a digital computer is just a network of switches that can turn each other on and off according to a set of logical rules. If a computer's switches start out in a pattern that represents, say, "2 + 2," these switches trigger changes that form a new pattern, which (if all goes well) represents "4." Such on-off patterns can stand for almost any instruction or result.

Making computers smaller and faster involves reducing the size of the switches and finding new ways of connecting them. Already, digital computers that once filled rooms and were crammed with wired vacuum tubes have evolved into etched scraps of silicon smaller than a fingernail. The size of individual circuit elements now begins to rival the wavelength of visible light. Nevertheless, a single circuit element still holds trillions of atoms, and a single computer chip remains visible to the naked eye.

Carter imagines a future, sugar-cube-sized computer with a million billion molecular "gates," compared with the million or so transistor switches laid down on the best present-day silicon chips. Switching speeds would be up to a thousand times faster than those in current supercomputers.

Molecules can behave like switches in several ways. One simple form is a molecular rectifier or diode, which allows an electron (or a "current") to travel along a chainlike molecule in one direction but not in the opposite direction. At the workshop, Robert M. Metzger of the University of Mississippi in University, Miss., described his attempts to synthesize such a rectifier. This involves inserting a molecular "bridge" between a molecule that readily donates electrons and one that is a good electron acceptor, a task more difficult than it sounds. Normally, electron acceptors and donors will react with each other directly, unless the reaction that forms the full chain is fast and efficient. That means selecting the molecular ingredients carefully.

Metzger reported that his group may have succeeded in building a molecular rectifier using a urethane bridge between the donor tetrathiofulvalene and the acceptor tetracyanoquinodimethane. But many obstacles remain. One problem is finding the best combination of molecular ingredients to form an efficient rectifier. Another is finding a way to mount the rectifiers as an organized, one-molecule-thick layer between two conducting metal films. And unless low voltages are used and the device is refrigerated, there is always the danger of "frying" the component organic molecules.

Another approach is to use photochromic crystals, which change color when they are irradiated. Hans Sixl of the Universitat Stuttgart in West Germany discussed research on the molecule salicylidene aniline. In its stable form, this substance is colorless, but it turns red upon irradiation with ultraviolet light. Visible light or heating returns the red crystal to its colorless form. At the molecular level, this reversible reaction involves the shift of a hydrogen atom from one part of the molecule to another.

Sixl pictured photochromic molecules as switches, inserted in long, chainlike molecular "wires" that conduct electrons or vibrational pulses (solitons). Shining light on a photochromic junction could alter the molecular structure enough to prevent the passage of an electron or soliton along the wire. A different color would restore the wire's conductivity.

The leading candidate for the role of "molecular wire" is the one-dimensional polymer trans-polyacetylene $(CH)_x$ (SN: 4/30/83, p. 284; 2/6/82, p. 90). With its backbone chain of carbon atoms joined by alternating single and double bonds, polyacetylene is an electrically conducting polymer. Electrons or solitons injected into these chains will propagate along the molecule. In a sense, the effect is similar to generating a pulse and seeing it move down a long, extended spring.

Another conducting polymer, sulfur nitride $(SN)_x$, has the advantage of bonding directly to a clean, metallic surface. Carter sees the possibility of growing sulfur nitride filaments, segment by segment, on silicon surfaces. Using this approach, perhaps a computer could be synthesized or grown in solution, he speculates.

Combining special-purpose molecules with molecular wires can produce most of the necessary circuit elements for a computer. Carter, for example, has assembled designs for memory elements, logic gates, soliton generators and other molecular electronic devices. Some arrangements, in which molecules can shift through three or more states rather than just two (representing "on-off" or "one-zero"), potentially can process information in logic systems other than the conventionally used binary system.

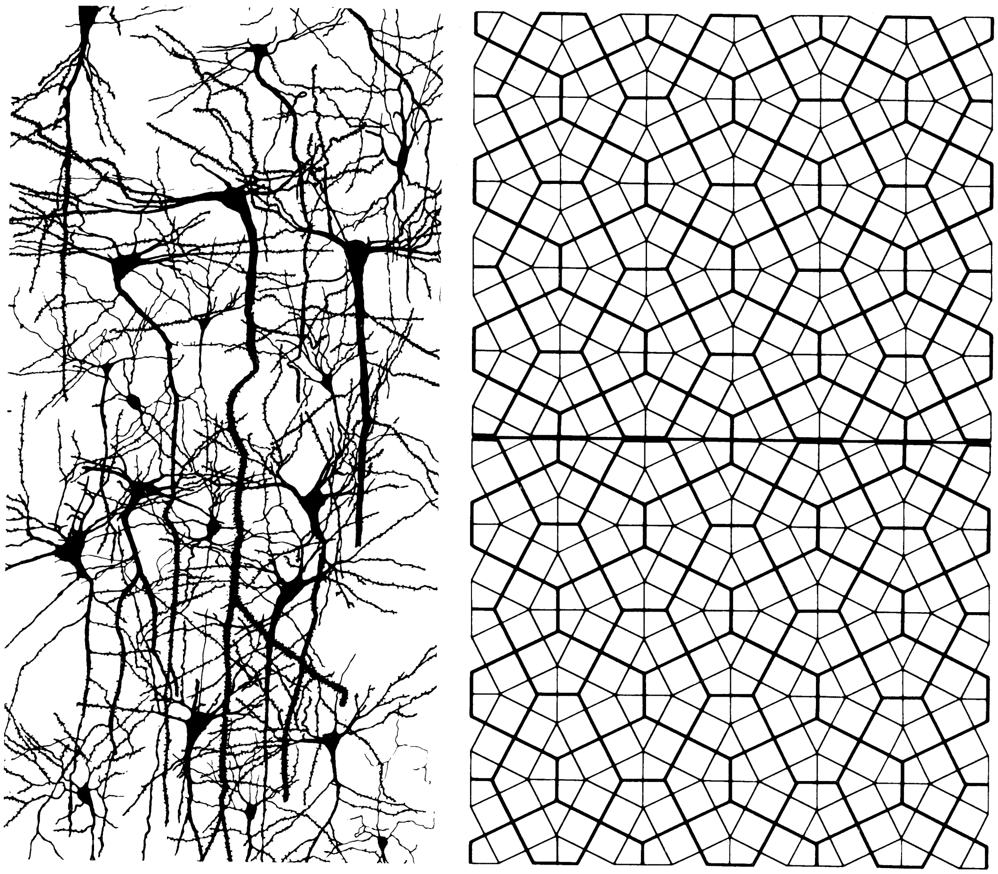
Most of the molecules discussed at the workshop have not yet been made. Michael P. Groves of the University of Adelaide in Australia, who also presented designs for soliton circuit elements, said the designs are useful because they give chemists an idea of what to aim for in building molecules. "Synthetic chemists must be encouraged to try to do them," Groves said.

Still, the task facing synthetic chemists seems overwhelmingly complicated and delicate. Carter, looking at one of his own designs, admits, "I really wouldn't want to make one of them."

One solution is to find a way for molecules to assemble and organize themselves. Hans Kuhn of the Max-Planck Institute in Göttingen, West Germany, works with molecular films more delicate than a soap bubble. His films (called Langmuir-Blodgett films), only one molecule thick, are made from substances similar to soaps or oils, which spread out on a water surface but do not dissolve. A glass slide immersed in the water and then pulled out emerges covered with a thin but surprisingly tough film. Kuhn showed how it was possible to construct films made up of layers of different molecules. He also described designs for optical switches that incorporate layers of light-emitting and light-absorbing dye molecules.

Kuhn compared this technique for building molecular electronic devices with the processes that led to the origin of life. The crucial process is the formation of a simple structure by interlocking appropriate molecules, he said, either within a film or between monolayers deposited one on top of the other. "Looking at making simple molecular devices could give hints of how simple molecules aggregated to form life," Kuhn suggested.

Instead of piling up a sequence of molecular layers, Kevin M. Ulmer of Genex Corp. in Gaithersburg, Md., suggested creating patterns within a single monolayer. Creating an integrated circuit pattern is like laying tiles on a floor, he said. Thus, it may be possible to force different protein molecules, for example, to crystallize into a complex mosaic pattern within a monolayer. Proteins, like insulin, are already known to crystallize in orderly, one-molecule-thick layers. Making a checkerboard pattern or something even more complicated should be possible by mixing proteins that crystallize in different arrangements, he suggested. Designing molecular circuitry as mosaics comes down to the task of building individual tiles and using monolayer techniques to assemble them, said Ulmer.



The "molecular computers" or brains of living creatures consist of a maze of neurons (left) with thousands of interconnections. As a first step toward building a molecular computer, some researchers propose laying down mosaic patterns of different crystallized proteins in one-molecule-thick layers. (Left: Reprinted by permission of Perigee Books, from The Brain: A User's Manual by The Diagram Group, ©1982 by Diagram Visual Information)

Many years ago, Richard P. Feynman of the California Institute of Technology in Pasadena, Calif., in a talk entitled "There's Plenty of Room at the Bottom," suggested another approach. Ordinary machines could build smaller machines that could build still smaller machines, working step-by-step down toward the molecular level. At the workshop, K. Eric Drexler of the Massachusetts Institute of Technology in Cambridge, Mass., discussed the use of molecular machinery to assemble molecular electronics. Instead of handling atoms in "thunderous herds" in bulk processes like melting, etching, deposition and organic chemical synthesis, molecular machines could build structures atom by atom. Specially designed molecular "tools" could act as templates, and could shift or assemble atoms, repair damage or correct errors. Already, genetic engineering techniques are pointing the way.

Drexler also noted that the switches in a digital computer do not have to be electronic. Hinged molecules, in which "arms" move like gears or levers, could be put together to create mechanical calculating machines, somewhat like the mechanical computers built during the nineteenth century (illustration, p. 378). Mechanical signals travel much more slowly than electrical signals, but, said Drexler, a calculating machine with molecular gears would be small enough to run as fast as today's electronic machines.

Even if a tiny computer can be built from molecular electronic devices and methods are found for eavesdropping on individual molecules so that information can enter or leave the computer, other fundamental problems remain. Robert O. Grondin of Colorado State University in Fort Collins pointed out headaches already encountered by designers in scaling down circuit elements on silicon chips. The difficulty is "parasitic coupling," he said. Individual circuit elements can no longer be considered independently. For example, if two transistors are laid down side by side, the area between the two transistors acts like a third transistor. The problem is not the total number of elements but the number of elements packed into a given space, Grondin said.

Grondin also said that circuit elements arranged in an orderly periodic pattern often act together in unforeseen ways. "In dense integrated circuits, individual devices or cells may behave differently in an array from the cell behavior in isolation," said Grondin. In addition, a small, local effect can be amplified into something that affects the behavior of the entire circuit. Designers must be aware of these interactions and design around them or use them, he said. For molecular devices, these interactions and "crosstalk" problems would be much worse.

Reliability is also an important issue. Radiation, including alpha particles and ultraviolet light, can easily alter and damage molecules. Random motion of the molecules, associated with heat, can cause faults too. Avoiding this would require a perfectly shielded and air-conditioned computer (which would no longer be small in size), or a design with sufficient redundancy so that an element failure would not shut down the whole system. For example, Grondin suggested that information stored as a pattern distributed throughout the memory rather than in one location would be less susceptible to random noise and error.

The obvious model for designing a molecular computer is the human brain. One puzzle, said Gilbert Baumann of Duke University in Durham, N.C., is how nature made such a reliable system out of unreliable components. The firing of nerve cells in the brain, for instance, seems to rely on seemingly random molecular events in the membranes that envelope cells. Yet the human mind, as a whole, can perform mental feats that no present-day electronic computer can match. But at the same time, computers can do certain restricted tasks far more precisely and quickly than a human being.

Paradoxically, it is conceivable that the attempt to scale down computer circuits to molecular size may require the same design considerations and compromises that produced the human brain. The computer may lose its precision and speed in favor of greater fault-tolerance and flexibility.

So far, Carter says, there has been lots of interest but only a small amount of work on molecular devices. "The ideas are coming fast, but the work to verify them is not coming as fast," he says. However, some of the tools needed to develop the necessary chemistry are just becoming available, he adds.

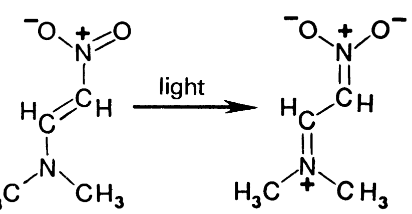
The workshop's keynote speaker commented, "We face formidable problems that may take years to solve, but the challenge captures the imagination." On the way, molecular electronics research may uncover new insights on how molecular systems function and on new technologies with applications quite different from any now imagined. □

Solitary pieces for molecular devices

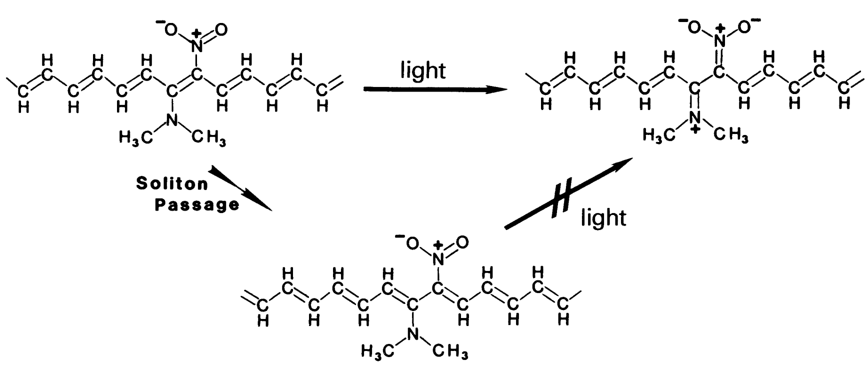
Solitons are solitary waves that can travel unchanged for long distances. Some researchers believe such single pulses can propagate along chainlike molecules such as polyacetylene, which consists of a chain of carbon atoms connected by alternating double and single bonds. Trans-polyacetylene has two possible configurations, depending on the positions of the double bonds. However, if a long chain contains both configurations, a "kink" occurs where the two different patterns meet. This disturbance, associated with a single electron that doesn't know quite where it ought to go, is one example of a soliton. The passage of a soliton along the wirelike polyacetylene molecule results in the exchange of single and double bonds. Scientists predict these solitons should be very mobile.

Forrest L. Carter, a Naval Research Laboratory chemist, suggests that these molecules can be turned into switches by inserting appropriate molecular groups at strategic points along the chains. For example, in a "push-pull" olefin, light absorption transfers an electron from the amine nitrogen at the bottom of the molecule to the oxygens at the top.

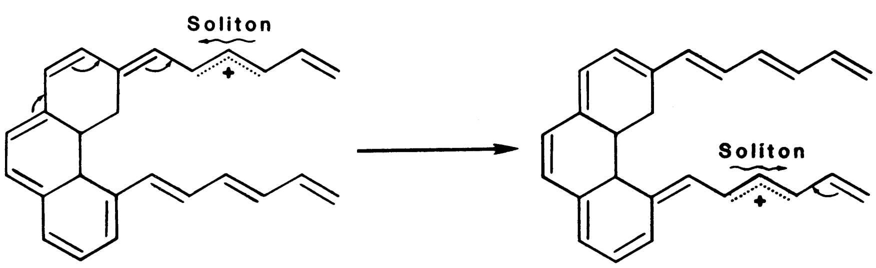
Push-Pull Olefin



When the olefin is embedded in a polyacetylene chain, light will be absorbed only if there is a double bond between the two carbon atoms of the olefin. When the passage of a soliton turns the double bond into a single bond, light cannot be absorbed because there is no path for electron transfer.



Carter has also designed molecular arrangements that, theoretically, reverse solitons and perform other functions needed in electronic circuits. Unfortunately, no synthetic chemist has yet built these molecules.



Illustrations: F. Carter, NRL