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'Moletronics' May Hold Key to Faster, Cheaper Computing Power

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In some ways, electrons barely seem to exist.

They've been described as "negative twists of nothingness." They're both particle and wave. Even gathered into atoms, they're only an amorphous probability, more likely to be found in one looping track than in another.

Atoms themselves—just electrons swinging around a cluster of neutrons and protons—seem scarcely more tangible.

Yet scientists control them. They push them around like pebbles, to shape letters and to spell out words. They coax them together to form molecules that can do specific tasks.

For example?

At Yale, engineer and Academy member Mark Reed, working with colleagues here and elsewhere, has developed molecules that can perform some of the jobs now done by the clumsy devices of silicon at the heart of your computer. What's more, these molecular devices show promise of performing more efficiently, more powerfully, and more economically than the silicon that they may soon replace.

Reed works in the field of molecular electronics, or moletronics. It's a field that was made possible only in the1980s, with the development of the scanning tunneling microscope. This tool can perceive individual atoms. Instead of a lens, it uses an atomic-size tip which can sense the electrical charges of individual atoms on the surface of an object. The tip travels over that surface, bouncing up and down in response to the charge. That movement is translated by a computer into a picture of the atoms.

The ability to work with individual atoms is a boon to fields from materials science to pharmacology. But to those who work with computers, it offers a way to skirt the increasingly onerous limitations of silicon. Silicon has served the field well of course, taking it from room-sized computers based on vacuum tubes to today's increasingly tiny and powerful processors. Right now, computers based on silicon continue to grow in power and drop in cost. Designers make computer chips more powerful by miniaturizing the devices—the transistors and switches—that hold the bits of information that enable the computer to remember and calculate. The smaller these devices get, the more designers can squeeze onto a chip, thus increasing its computing power. The famous Moore's Law holds that the number of transistors on a circuit would double about every 18 months. Since 1965, when this prediction was made, it has proven accurate, but most believe that it will not continue to hold true much beyond 2015.

As designers crowd devices closer and closer together, the chips become far more expensive to produce. Right now, a chip can hold about 42 million transistors, but, because of increasing precision and quality control this kind of density requires, a chip fabrication plant ("fab") now costs over $1.5 billion. This amount will certainly grow, and many estimate that by about 2015, new fabs will be too expensive to justify.

But even if cost were not a factor, there's a physical limit to the performance that silicon can achieve. Currently, engineers are able to shrink these devices to about 180 nanometers. But researchers estimate that they can't be made much smaller: At less than around 50 nanometers, silicon devices begin to lose their ability to hold information.

The devices constructed by Mark Reed and his colleague James Tour, a chemist at Rice University, are based not on silicon but on a ring-shaped molecule known as benzene. Like traditional devices, these molecular devices process information by controlling electricity. Both kinds have the ability to turn a flow of electrons on and off, to control the direction of the electrons, and to store electrons. But they do this in very different ways.

Silicon is a semiconductor, which means that under certain conditions, the bonds that hold the atoms together are freed (by inserting a few, very dilute concentration of different atoms other than silicon, a process called "doping"), allowing electrons to freely move through the silicon. Benzene, though, is an organic molecule, and typically organic molecules, which contain carbon, do not conduct electricity. That's because carbon tends to bond to itself and other atoms in covalent bonds—very tight bonds, which hold electrons firmly in place—and the concept of doping no longer holds.

Benzene, though, is different. Its ring of six carbon atoms (with a few hydrogen atoms thrown in as well) is held together in part by a pi bond—a sort of smeared bond in which some of the electrons are loosely shared by all the atoms in a kind of cloud that circles above and below the carbon ring. It's not a broken bond. Instead, it's a sort of bond within which electrons are somewhat more able to move.

Mark Reed and James Tour began working together in 1991. It took about five years to demonstrate that their concept could work. "The initial structures," says Reed, "were simply to show that indeed you could have electrical contact with a single molecule, and that you could pass currents around." By 1997, Reed was able to hold a single molecule between two tips of a specially designed scanning tunneling microscope, and measure the current it carried, finding that in fact the molecule could handle a far greater magnitude than anyone had expected.

But that was only the beginning. To make moletronic computers a reality, the devices had to do more than merely let electrons flow through them. They had to control that flow.

So, says Reed, "we made the molecule more interesting." They began to synthesize molecules that could serve as active devices. "We made the molecule longer," explains Reed. "We added additional benzene rings, and put various endgroups on it."

By changing the structure of the molecule, the researchers found that they were able to alter its behavior. They hung molecular fragments—an NH2 group and an NO2 group—from the middle benzene ring. This distorted the electron cloud, making the molecule more susceptible to twisting. By applying a voltage to the molecule, for example, they could cause a "change, a bend or a twist in the molecule." This disrupted the flow of electrons. And, this twist was reversible. When the voltage was removed, the molecule returned to its original shape, allowing current to pass through once again. In other words, this molecule can act as a switch. It turns electricity on and off—a basic characteristic that a computer needs to process information in bits of 1 and 0.

Importantly, the researchers have also been able to design a molecule that stores those bits—a molecular device that is able to act as a memory.

When Reed and his colleagues create these molecules, he jokes, "there's a big Edisonian component involved." The field is so new that the physics of what happens is not really yet well understood. Only recently, he explains, have theorists had to grapple with the idea of current passing through a molecule. "We're rewriting the book on what molecular models might look like where there's a high electric field and a current passing through." They do have a few basic principles that they work with. "You know what kind of groups will give you high conductivity through the structure. You design it with groups that have a high degree of electron mobility." But they can't yet design a molecule from scratch, and know without testing how it will behave.

Reed does the testing, analyzing and characterizing the molecules synthesized by Tour. "I incorporate it into the device, I put electrical leads on it, I measure the electrical transport current vs. voltage characteristics, I subject it to various types of tests like temperature, to understand its energy states."

Often, he says, they will analyze a structure for a few months, to understand all aspects of the transport. "It's an investigative job," he says, "It's really tearing it apart to understand the basic structure going on in there. If you don't keep your eyes open, you'll miss something."

In fact, it was just that attentiveness led him to notice the molecule that may become the first moletronic device to be incorporated into everyday life. It's a memory device. Like a switch, it can either transmit current, or block it. But rather than using molecules that twist and untwist, it relies on molecular fragments, such as the NO2 group, to trap electrons. Depending on how the electrons are trapped, the molecule transmits current (a binary 1) or blocks it (a 0 bit). And, in a notable improvement over silicon memory, the molecular device is able to store information for about 15 minutes.

"We stumbled across this memory effect because we noticed an approximately 3 percent change in one graph," remembers Reed. One of his students, he said, showed him some of her data, and he noticed that one of the measurements—the second—was just slightly different from all the others, which were all the same. Typically, the very first measurement was not kept, but in this case, Reed had the experiment redone so that he could go back to look at it. "It was dramatically different," he says.

"We tore that apart for about a month or two," he says. But finally they realized that the later measurements were stable because the device was storing charge, while the first measurements differed because device was still in the process of being charged up. In fact, they had the basis for a memory device.

"We finally figured out what was going on, and then we went and enhanced it. We found that if we did it right, we got a huge memory effect. You have to keep your eyes open."

It's that serendipitously discovered device that's expected to be the first to come to market, developed into a commercial product by the Molecular Electronics Corporation, a company founded by Reed, Tour, Dave Allara and Tom Mallouk at Penn State, and Brosl Hasslacher at Los Alamos Labs.

People often assume, says Reed, that because you have a certain new technology, immediately what you're going to do is make a supercomputer. But supercomputers are not the only way to take advantage of nanodevices. For one thing, even though researchers have recently reported constructing simple molecular circuits able to perform some calculations, the practical barriers to realizing these computers remain huge. But molecular memory devices can be used now, in conjunction with the chip technology currently available.

Molecular memory devices, explains Reed, offer many advantages over conventional silicon devices. Their ability to hold memory longer is clearly significant. Silicon memory devices retain charged bits for only a millisecond before the charge leaks away. That means that each piece of information must be restored ten to a hundred times a second, which requires substantial amounts of power.
Because Reed's device retains its electrons for about nearly fifteen minutes, it has, he explains, "the ability to get information in and out using significantly less power. Compared to, say, current equipment, which only runs for a few hours before the batteries wear out, Reed says, machines using molecular memory could run for a week.

There's an energy structure, says Reed, that explains how long a device—either silicon, or molecular—will hold electrons. "They leak out at a certain rate," he explains, "and when you go to a molecular structure, the energies [holding the electrons in place] become much bigger. So the leak-out rate is slower."

Reed and his colleagues hope to synthesize molecules that can serve as even stronger electron traps. But even the memory that they have in hand will serve many uses, believes Reed. "While it isn't something that can sit on your desk for two weeks and then you come back to it, for many applications, 10 to 15 minutes of memory is all you need, because by then, all the calculations will be done." It will, he says, dramatically reduce power requirements, and he believes that it could have applications in virtually all portable electronic systems.

But the second advantage, says Reed, is that "the fabrication technologies for this are potentially very attractive from a cost standpoint." Unlike silicon, these nanodevices do not require costly manufacturing facilities. Instead, they rely on a process called "self-assembly." The molecules are designed so that one end will stick to a metal surface (typically, the contact is gold, says Reed). When the metal is dipped into a beaker of the molecules, the devices automatically attach themselves in their proper places. The process bypasses the need for fabs, and, between the ease of self-assembly and the drop in power requirements, "it has the potential," says Reed, "of doing electronics too cheap to meter."

Reed expects that his company will have a prototype ready in a year or two. It will, he says, make use of current technology by integrating the molecular memory devices into a standard silicon chip. They'll create a chip, using standard lithography processing, up to the point where the molecules must be absorbed. "Then we stick them in a beaker, and they self-assemble, just where we need them to be."

At this stage, they don't plan to use the molecules one at a time. "Scientifically, we can do a single molecule," says Reed. "But from a manufacturing standpoint, it's kind of silly." Instead, they'll be assembling four to five thousand of the devices on each 1 square micron spot, so that the molecules will act in a kind of tandem. This allows the researchers to bypass many of the problems inherent in working at such a tiny scale: for example, they won't need to design a wiring system minute enough to connect to one molecule at a time. Instead, they'll be able to connect the clumps of molecules with lithography wiring techniques currently in use.

Designing a system that incorporates molecular devices as working memory will be impressive enough. Yet that's probably only the beginning. Eventually, nanodevices could free computing from the constraints of silicon. "We could print this kind of electronics on a flexible film, like saran wrap, a few thousand feet a minute," says Reed. "I can incorporate simple communication circuits into clothes." Imagine, he says, wearing flexible computers that constantly fine-tune your environment for you: when you walk into a room, they'll automatically communicate and interact with the room: you will become part of the web of the room.

Fanciful? Maybe. There's still plenty of technology to be worked out, of course. But in fact, the field is advancing faster than anyone predicted. After all, who would ever have believed that researchers could pick up a single molecule and move it around? And who would have believed that individual molecules could be designed to work as devices? But they can. Like so much else, it's not just science fiction any more.—***Karen Miller***

[Karen Miller is a science writer based in northeastern Connecticut. Her articles have appeared in Northeast Magazine, and on the Science@NASA website.]

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