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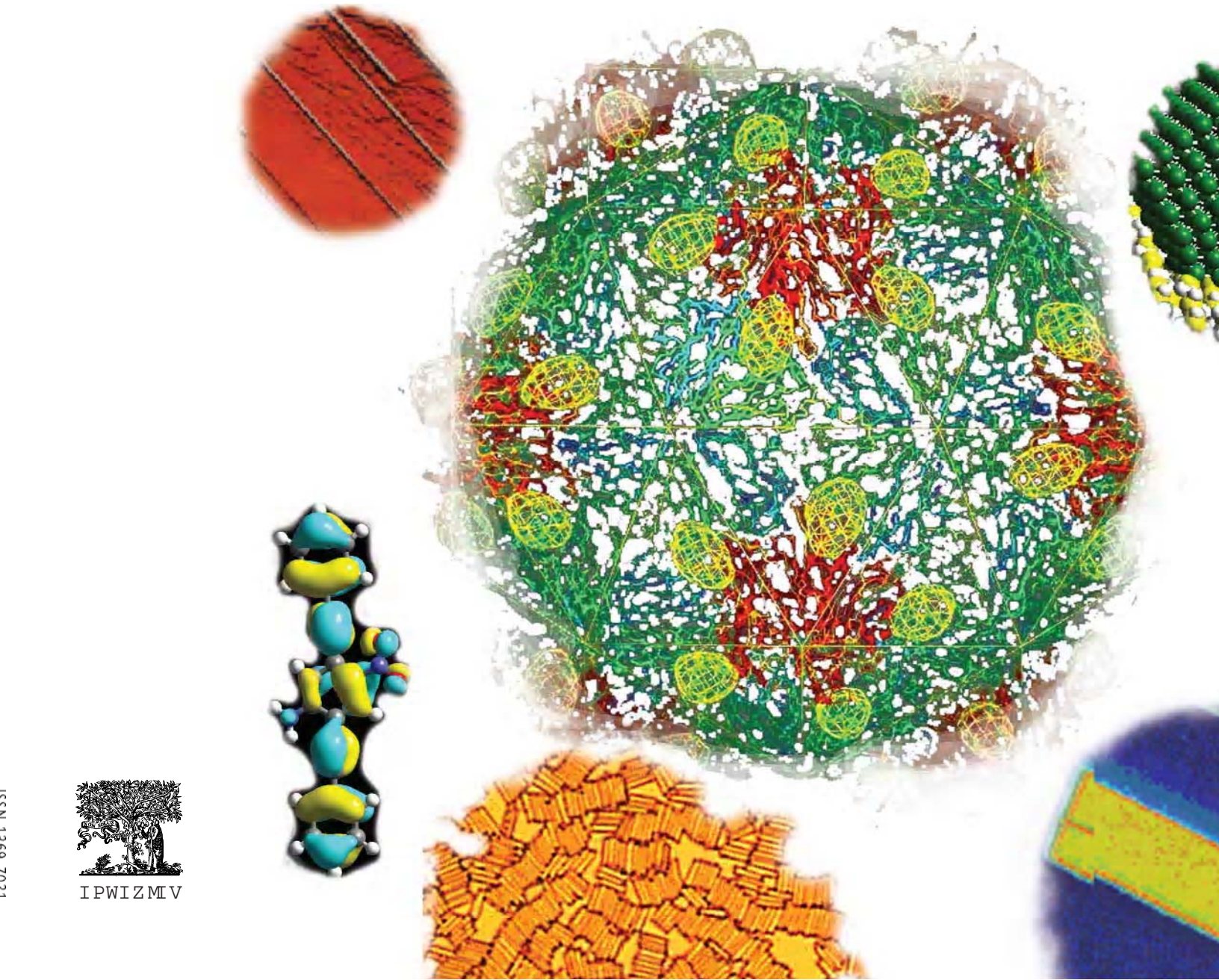
Molecular electronics - the future of computing



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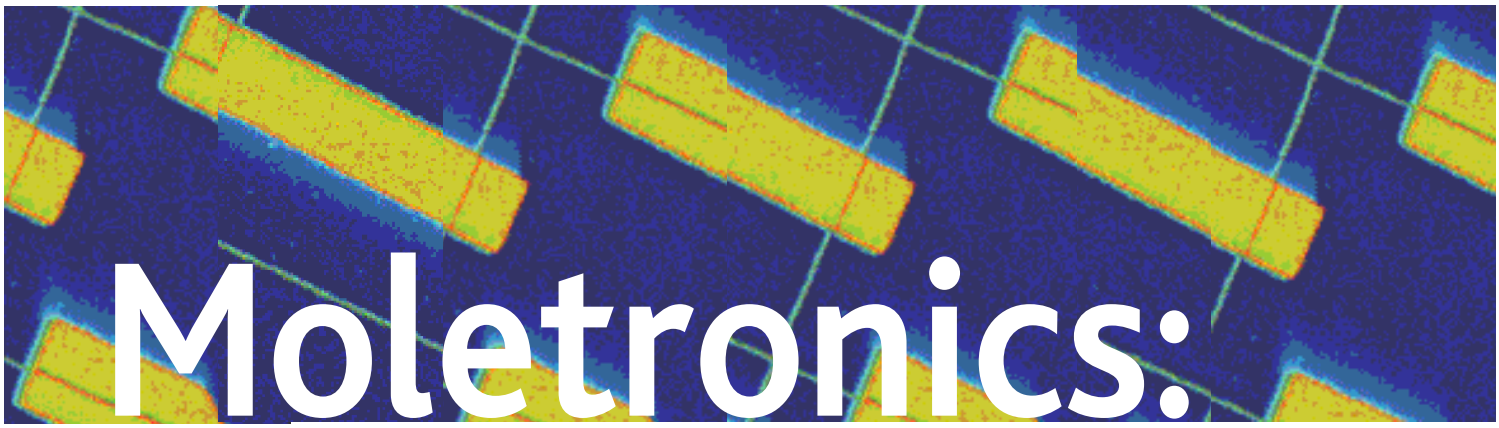

Moletronics: future electronics

by Kwan S. Kwok and James C. Ellenbogen*

Over the past several years there have been dramatic advances toward the realization of electronic computers integrated on the molecular scale. First, individual molecules were demonstrated that serve as incomprehensibly tiny switches and wires one million times smaller than those on conventional silicon microchips[1-4]. This has resulted very recently in the assembly and demonstration of tiny computer logic circuits built from such molecular-scale devices[4-10].

A major force responsible for these revolutionary developments has been the molecular electronics or 'Moletronics' Program organized by the US Government's Defense Advanced Research Projects Agency (DARPA). Previously, DARPA gave birth to the Internet in the 1970s and 1980s, revolutionizing the way the world communicates. Now, the agency is setting its sights on a new revolution in the nature, structure, and scale of the very materials with which the world both computes and builds. Ultimately, to compute with molecular-scale structures – i.e. nanometer-scale structures – one must learn how to characterize and organize them on similar scales, one by one and in vast arrays. This is creating a whole new science and industry of 'nanostructured materials', such as are portrayed in Fig. 1.

By using small aromatic organic molecules, carbon nanotubes, biomolecules, or semiconductor nanowires (Figs. 1 and 2) to enhance or supplant conventional bulk silicon, DARPA sees the potential to put as many as a trillion electronic switches in a square centimeter. This would permit, for example, a computing system that contains approximately 10 billion switches to be fabricated on the top of a grain of salt.

To understand what a giant step this would be beyond today's electronic computers, one needs to appreciate that a conventional commercial microcomputer chip still contains only about 10-50 million switches in a much larger area, the size of a large postage stamp. That is, Moletronics is planning for a computer with devices and circuitry as much as one

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million times denser than that in today's state-of-the-art commercial microcomputer. This would address concerns expressed in the electronics industry about the difficulties that may be encountered in the further miniaturization of conventional silicon semiconductor microelectronics[11-14]. Beyond that, though, it is envisioned that the large quantitative change in the density of computation using molecules is likely to be accompanied by dramatic qualitative changes in the nature and applications of computation. Computation literally would become a property of matter.

DARPA's Moletronics Program has mapped out and is succeeding in following a pragmatic step-by-step approach to achieving this radical vision for future electronic computers. Among the primary goals for the program are to develop functioning prototype electronic computer processors and memory integrated on the molecular scale. Already Moletronics has been successful in building and challenging a community of investigators that have succeeded in demonstrating a variety of molecular-scale switching devices, circuits, and the techniques for their assembly. Also, these investigators have made major contributions[5] to the several very recent dramatic advances[4] in research toward the realization of electronic nanocomputers.

Especially exciting is the fact that second-order impacts of all this research already are appearing in important experiments being conducted outside the Moletronics Program[8,9], which are adopting its concepts, devices, and fabrication techniques[15-20]. However, the Moletronics Program is committed to much more than promoting research. It is committed to building actual prototype molecular-scale electronic computing systems that will produce a quantum jump in the concept and the commerce of computation, thereby sowing the seeds for a revolution in materials science, as well as in electronic computation.

The physics is with you

From a materials perspective, the heart of this impending revolution is the discovery of new physical phenomena in the mid- and late-1990s. Individual molecules, such as those depicted in Fig. 2, were shown experimentally to have electrical properties that previously were thought to occur only in bulk semiconductors. This is extraordinary because each of these molecules is only a few billionths of a meter long. As recently as 1996, it was an open question whether individual molecules such as these could conduct electricity.

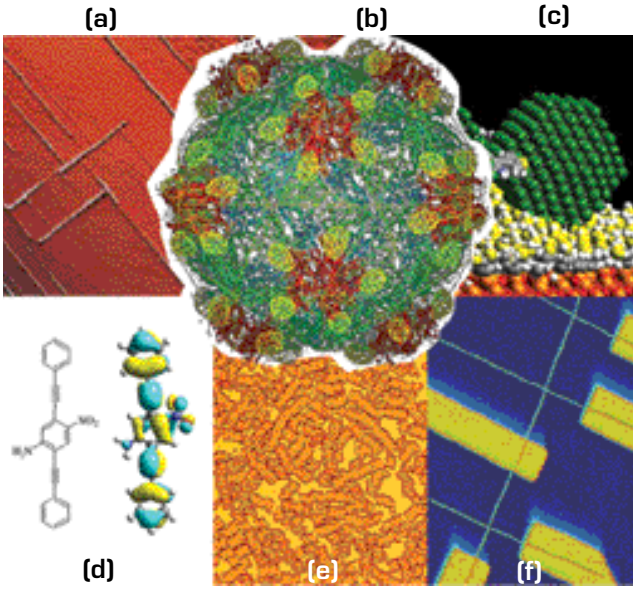

Fig. 1 Moletronics nanostructured materials. (a) Electron micrograph of self-assembled $ErSi_2$ nanowires developed at HP. (Reproduced with permission from[54].); (b) electron micrograph of cowpea viral particle modified with gold nanoclusters developed at NRL to use as a template for molecular self-assembly; (c) simulation of Rice University's gold-nanoparticle electrical contacts on a surface in a 'NanoCell' molecular logic structure[51]; (d) structural diagram of NDR diode switch molecule[20,28,35] and a simulation of its molecular orbitals involved in switching. (Reproduced with permision from[47]. Copyright 2000 American Chemical Society.); (e) gold nanobars synthesized at PSU; (f) electron micrograph of nanowire transistor-based logic circuit[4] that was self-assembled and demonstrated at Harvard University. (Reprinted with permission from[5]. Copyright 2001 American Association for the Advancement of Science.)

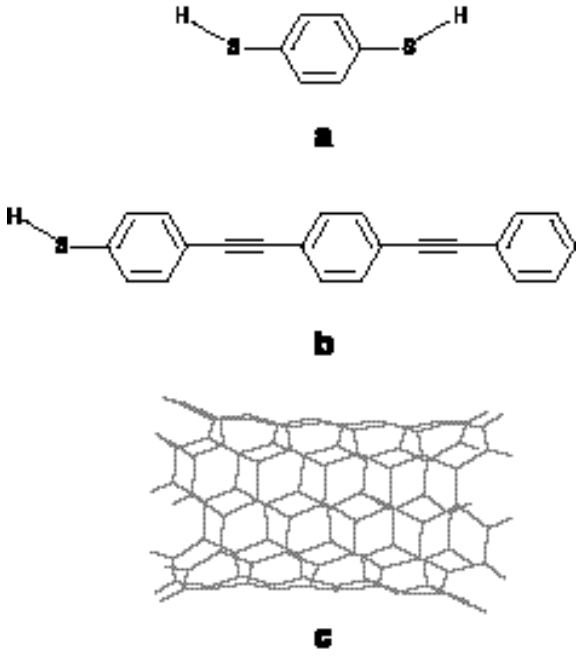

Fig. 2 Conductive molecular wires. Schematics of molecular structures for (a-b) conductive polyphenylene-based Tour wires[15-19,22] and (c) a carbon nanotube[23,24].

Table 1 *Conductances of molecular wires expressed in appropriate nanoscale units compared with the conductance of a macroscopic copper wire expressed in the same units*[1].

Device	Cross-sectional area (nm^2)	Current density (electrons/nm^2-sec)
1 mm copper wire	~$3x10^{12}$	~$2x10^{6}$
Polyphenylene Tour wire	~0.05	~$4x10^{12}$
Carbon nanotube	~3	~$2x10^{11}$

This issue was settled by a series of important experiments in the period from 1995 through 1997[16-17,21-24]. Very soon thereafter it was shown that individual molecules also can switch small electric currents[18-19,25-28].

While these currents are small in absolute magnitude, their densities are enormous. As many as one trillion electrons per second pass through a single square nanometer each second in these monomolecular semiconductors. Using appropriate nanoscale units, the current density through small polyphenylene molecules, such as those depicted in Figs. 2a and 2b, or the carbon nanotube depicted in Fig. 2c, is approximately one million times as great as for a 1 mm diameter copper wire (Table 1)[1].

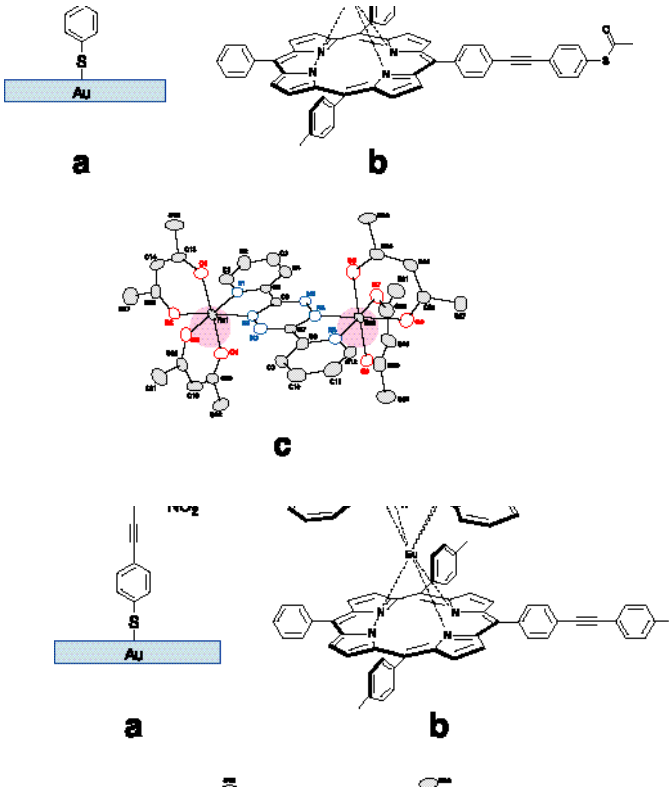

Fig. 3 Memory molecules that store bits and states. (a) Programmable/erasable polyphenylene-based switch used by Yale-Rice-PSU Moletronics team in molecular RAM cell. (Reproduced with permission from[36].); (b) porphyrin multi-bit memory cell by UC-Riverside-NCSU Moletronics team[69] (Reproduced by permission of The Royal Society of Chemistry.); (c) ruthenium-based dimer being used in efforts at Notre Dame University to build and demonstrate molecular QCA memory and logic[79]. Reproduced with permission from[78]. Copyright 2001 American Chemical Society.)

Some of the monomolecular switching effects that have been observed are unexpectedly large, as well. The precise mechanism of such robust switching on such small scales remains something of a mystery. The fact that it occurs, however, has been verified in a number of experiments[6-10,20,29-36]. This, along with the robust phenomenon of monomolecular conductance, means that the physics strongly supports efforts to make molecular-scale computer circuits and systems.

In a related paper appearing in this issue, Moletronics investigator Mark Ratner provides an overview of some of the structures and mechanisms for conductance and switching in molecules[37]. These also are discussed in greater detail elsewhere[1,2,38-41].

Strong collaboration

Within the Moletronics Program, several interdisciplinary teams are pursuing complementary, mutually supportive approaches to exploiting the favorable physical and chemical properties of molecules to make nanocomputers. The teams are experimenting with a range of structural, architectural, and assembly strategies.

Closely associated with the above-mentioned experimental breakthroughs in monomolecular wires and switches was an interdisciplinary team of investigators in a collaboration between Rice University, Yale University, and the Pennsylvania State University (PSU)[42]. Led by James Tour, Mark Reed, Paul Weiss, and David Allara, this team now is one of the linchpins of the Moletronics research and development effort. Developing further on its work, the team has taken steps toward understanding and improving the junctions between metal contacts and molecules[43-46], as well as the operation of insulating, conducting, and switching molecules[20,47-50]. One such switching molecule, plus the molecular orbitals that switch the current, is shown in Fig. 1d.

Applying insights from earlier device experiments, the Rice-Yale-PSU investigators are exploring a novel 'random assembly' strategy for building logic circuits. This strategy takes advantage of the way molecules naturally tend to arrange themselves on surfaces in implementing a type of programmable molecular logic array termed a 'NanoCell'[51].

Still further, team members have shown recently that molecular switches, like the one depicted in Fig. 3a, also have properties that can be applied to store information electrically and to build memory systems[36], which is a major goal of the Moletronics Program.

Another linchpin of the Moletronics R&D effort is an interdisciplinary team led by R. Stanley Williams and Philip J. Kuekes of Hewlett-Packard Corp. (HP), along with James R. Heath and J. Fraser Stoddart of the University of California at Los Angeles (UCLA). Their contribution to the Moletronics Program starts with a comprehensive, defect-tolerant architectural approach which is based, in part, upon much earlier experiments at HP with macroscopic, large-scale, defect-tolerant computing designs[52,53]. As has been emphasized by this team, defect tolerance is likely to be essential to any computer system design which anticipates having as many as one trillion switches and wires – especially one which will rely for its manufacture on such intrinsically statistical processes as molecular self assembly.

The high-level HP/UCLA design has been filled in piece-by-piece with novel molecular-scale electromechanical switches[30-32] (Fig. 4), techniques for fabricating nanowire structures via self-assembly[54-56] (Fig. 1a[54]), and a design for nanoscale 'crossbar' wiring harness[53] (Fig. 5a). This design concept includes strategies for external control and communications, as shown in Fig. 5b[57], as well as for interconnection[58], that are adapted to a molecular-scale computing structure. This has led to groundbreaking molecular computer circuit demonstrations[29]. These innovations are part of the HP/UCLA team's systematic industrial plan for building and manufacturing molecular electronic computers[53,57,58]. Following this plan, the HP/UCLA team has built and demonstrated a 16-bit molecular crossbar memory array that incorporates 16 molecular diode switching nodes[59].

A key Moletronics team led by Charles Lieber at Harvard University started out with the goal of exploiting the novel electronic and mechanical properties of carbon nanotubes for computation. It made considerable progress in that direction[33]. Recently, however, the team made breakthroughs in using molecular-scale semiconductor nanowires for building nanoscale wiring systems[60] and transistors[61], assembling them into a complete set of logic circuits with very robust switching characteristics[5]. One such nanowire logic circuit is shown in Fig. 1f. A fundamental advance in this

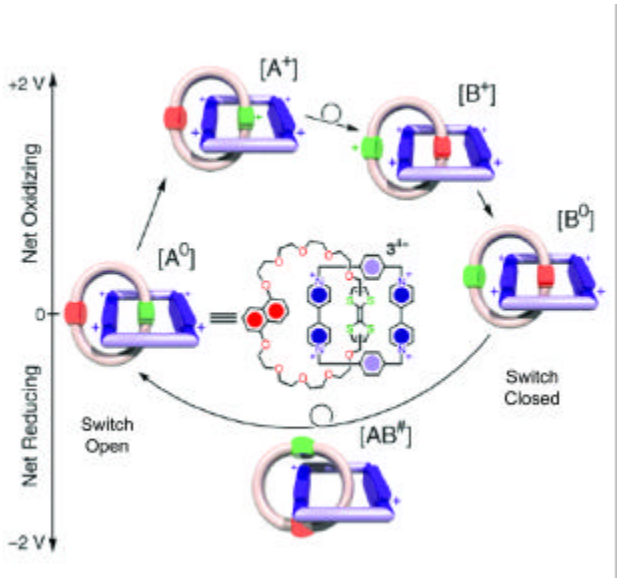

Fig. 4 Molecular electronic catenane switch demonstrated at UCLA closes when one of linked molecular rings rotates due to application of an oxidizing potential; switch is reopened when reducing potential is applied, rotating the ring back to its original position[32].

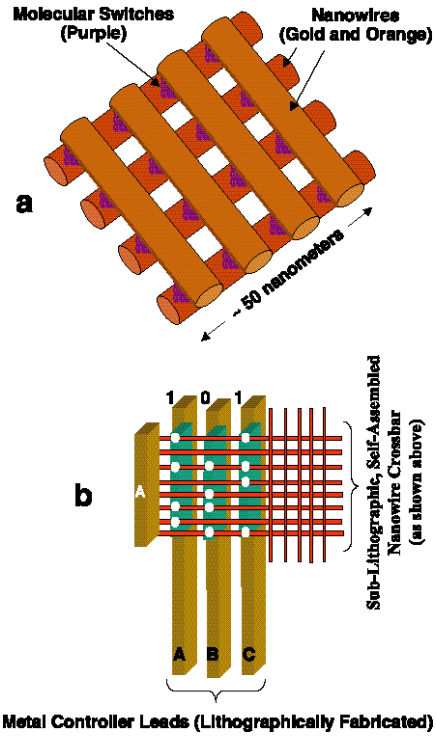

Fig. 5 (a) Molecular-scale crossbar circuit architecture devised by HP/UCLA Moletronics team[53] sandwiches switching molecules between crossed nanowires; (b) demultiplexer for a molecular memory network[57] that is built with the nanoscale circuitry in (a).

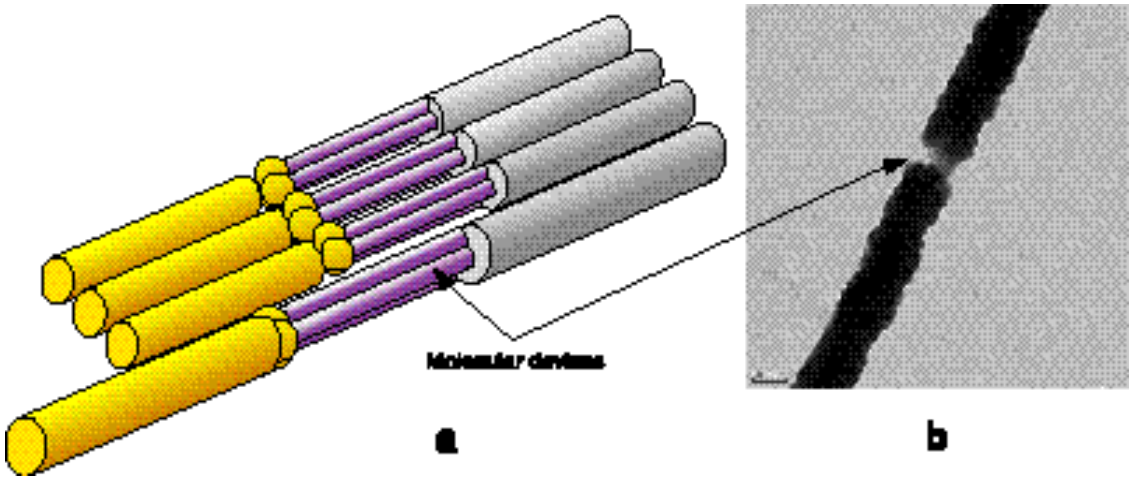

Fig. 6 Molecular devices built into nanowires by PSU Moletronics team shown (a) schematically and (b) in an electron micrograph of two 50 nm diameter nanowires with molecules embedded in the joint between them.

work was the development of a crossed nanowire transistor, where all of the nanometer scale metrics are defined by the nanowire building blocks and by 'bottom up' assembly – not by conventional 'top down' lithography.

More recently, Lieber and Harvard Moletronics team collaborator Hongkun Park have taken a significant step forward in their work toward development of high density memory. By exploiting the unique properties of chemically-distinct nanowires, which permit these varied building blocks to be combined seamlessly via a bottom-up assembly strategy, they fabricated a nonvolatile, bit-addressable, crossed-nanowire memory structure. Memory cells only 5 nm on side have been demonstrated.

The Harvard team's step away from nanotubes to apply nanowires for computation epitomizes the high quality of the science that is practiced throughout the Moletronics Program. Lieber and his collaborators let the results they observed in the laboratory lead them on a less traveled path away from the fascination of carbon nanotubes. This avenue was dictated by the team's discovery of unexpectedly favorable chemistry for making and manipulating semiconductor nanowires, as well as unexpectedly favorable physics for transporting and manipulating electrons with them.

By contrast, carbon nanotubes, which are extremely conductive and about 20 to 40 times smaller in diameter than the nanowires, are notoriously unreactive, insoluble, and difficult to manipulate chemically. The Lieber team's unorthodox exploitation of nanowires may have significant industrial consequences. The techniques they have pioneered for making molecular-scale switches and circuits appear to be very reliable and scalable for making many nanostructures rapidly, with high precision and reproducibility. Plus, the same techniques are showing significant promise in application areas other than electronics, such as nanophotonics and bionanotechnology[62,63]. Lieber discusses some of these developments further in a recent article in *Scientific American*[64], as well as in an interview in this issue of Materials Today[65].

Another team that is enjoying significant successes with nanowires is led by Theresa Mayer and Thomas Mallouk at PSU. They assemble nanowires by lateral non-covalent interactions into two-dimensional bundles that form in surface wells patterned on silicon by photolithography. A large number of such nanowires are shown in Fig. 1e.

A hydrophobic/hydrophilic self-alignment technique has been developed for the purpose of bringing pairs of nanowires together to form crossed-wire arrays. This independently conceived approach is also unique in that it depends upon structures that embed small molecules with unique electrical properties tailored for logic and memory functions into gaps and junctions between nanowires. This is depicted schematically in Fig. 6a, while an electron

micrograph of molecules embedded in a nanowire is shown in Fig. 6b. The Mayer-Mallouk PSU team recently collaborated with Tour and Allara to apply this embedding technique for refined, in-wire demonstrations of molecular diode negative differential resistance (NDR) switches, like the one in Fig. 1d, first developed by Chen et al.[28,35]. The technique permits the molecules to exhibit unprecedentedly sharp NDR switching transitions at room temperature. Additionally, the PSU approach has facilitated large-scale organization of short lengths of nanowire into prototype computing arrays.

All these ideas for building molecular-scale electronic systems fulfill the vision of Ratner, who is a co-author of the first scientific paper on molecular electronics, written back in 1974[66]. Now, he has become the Moletronics Program's resident expert on the mechanisms of molecular conductance and switching[38,39,67]. He is also collaborating with a team from the University of Colorado at Boulder, led by Josef Michl, who is experimenting with one of the most daring design and fabrication strategies in the program: an effort to make and operate an entire transistorized logic circuit within a single molecule.

The Colorado group, which also is collaborating with groups outside the Moletronics Program from IBM and Brookhaven National Laboratories, already has succeeded in demonstrating three-terminal gating in a single small, 'channel' molecule using a nearby aluminum wire as a gate. Now Michl's team is seeking a sufficiently insulating molecular group to permit the incorporation of this gate, as well as the channel of a field-effect transistor (FET), into a single small molecule, as sketched in Fig. 7a.

This approach is aligned with designs for monomolecular circuits conceived independently by another team of Moletronics investigators at the MITRE Corporation[1,68]. One of these designs is shown in Fig. 7b. The approach taken by MITRE introduces the important idea of using intramolecular dopant groups to embed devices into molecular wires, an idea which already has been exploited by other Moletronics teams to make monomolecular diode switches[28,35,36]. It also should be useful for making monomolecular FETs[68].

Biomolecules are another major class of molecular structures that are being exploited for moletronics. This is essential to gain leverage from scientific investments in biotechnology that are providing highly refined ways of manipulating such molecules. Also, some classes of biomolecules, especially porphyrins, like cytochromes and

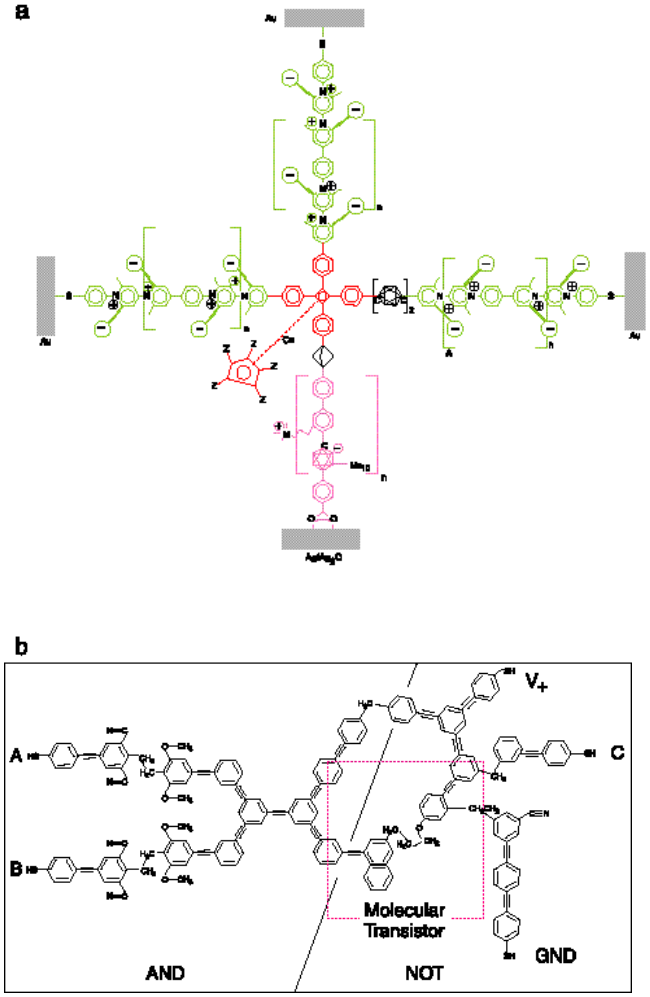

Fig. 7 Designs for monomolecular logic circuits due to Moletronics teams at (a) the University of Colorado and (b) the MITRE Corporation[68].

chlorophyll, are known to be very effective in storing and transferring electrons in nature. In fact, porphyrin-based molecules, like the one illustrated in Fig. 3b[69], are prominent elements of a highly developed molecular electronic memory system that is being fabricated by a Moletronics team led by David Bocian of the University of California at Riverside, along with investigators at North Carolina State University (NCSU)[69-71]. This memory system exploits the fact that porphyrins can store multiple bits of information in a single location, and that these can be accessed at voltages much lower than those needed for semiconductor memories.

Biotechnology also is being employed in groundbreaking and imaginative experiments for the assembly of Moletronics'

circuit systems. Biochemistry and biomolecules are uniquely evolved for imposing structure upon molecular materials. Nothing illustrates this better than the experiments led by Ranganathan Shashidar at the US Naval Research Laboratory (NRL) that use cowpea virus particles as the backbone for molecular memory and logic circuits. This cowpea-virus backbone is shown in Fig. 1b, where it knits together surrounding elements of the Moletronics Program in much the way it is being used at NRL to attempt to knit together small aromatic organic molecules that are to be the subunits of molecular computer logic and memory circuits. Already NRL investigators have mastered the technique for changing the viral DNA to grow large numbers of viral particles with multiple, site-specific modifications suitable for assembling conductive gold contacts on the desired surface regions of the particles. They have developed a faster technique for testing the conductance of molecules, as well, and used this to perfect conductive molecular devices to self assemble onto the gold-studded viral particle.

Generating a rising tide

The different teams and specialists within the Moletronics Program are intended to provide a complete set of skills and techniques for building a molecular computer. To this end, strong collaboration and sharing of techniques is fostered among all the Moletronics teams. Often, after an idea, structure, or method is pioneered and proven by one team, it is adopted by other teams, and applied in new, sometimes unanticipated, ways. Thus, the succession of advances from each of the Moletronics teams, as well as from molecular electronics research teams outside the Moletronics Program, has produced a rising tide that lifts all boats.

Following a synthesis of the different approaches evolved through the collaborative process described above, the result is expected to be a revolution in the nature of the materials that will be used for future electronic computers – from bulk conductive materials to molecular-scale conductive materials. This revolution should take electronics beyond the limits of bulk inorganic silicon, transitioning it in stages, first to a 'hybrid' technology that uses nanowires or carbon-based, organic molecular devices in combination with bulk-silicon-based devices. Then, this may evolve to an all-organic molecular-scale technology. Note, however, this is not the same as the bulk organic semiconductor technology that is attracting so much attention at the moment, but the introduction and application of nanostructured organic materials, each molecule of which is an electronic device.

Scaling up on the nanoscale

DARPA's program pulls together all the diverse device and fabrication strategies described above in its drive to build, from molecules, a large-scale, ultra-high-density memory in a vanishingly small area. The theoretical densities possible for molecular-scale devices, such as the previously mentioned crossed nanowire circuits, are approximately one trillion bits stored per square centimeter[1,5]. By 2004, program plans call for the fabrication and operation of a 16 kilobit molecular memory array.

To fabricate memory arrays approaching the high theoretical density limit for molecules and molecular-scale nanostructures, moletronics is attempting to take advantage of novel chemical properties and processes for molecules, such as self-assembly[5,18-20,42,51,54,59,60,72], as well as their novel electrical behaviors[5,8,9,28-33,35,36,47,49,55,59,61,69-71,73]. Further, it is believed that ultimately this could result in a significant reduction in the manufacturing cost of commercial electronics.

For example, in addition to the above-mentioned NRL biomolecular self-assembly research, low-cost inorganic self-assembly is being used at HP to make extended arrays of erbium silicide wires (Fig. 1a) to serve as high-density scaffolding for nanoscale molecular switches[54]. Other Moletronics research groups that have made similar or related advances include those at PSU, Rice University[72], Harvard[6,60], and UCLA[59].

Many of the same strategies that are being applied to the fabrication of molecular memory arrays also apply to molecular-scale logic. Several research groups in the Moletronics Program have demonstrated logic circuits made from molecules and other molecular-scale structures[6,29].

The high theoretical density possible for molecular-scale devices is likely to present new problems for extended circuit systems. At the very least, it could exacerbate system problems that already are significant in less dense microcircuits , such as dissipative heating and slowdowns that result from the proliferation of interconnects with high capacitances.

With respect to these issues, a number of innovative architectural approaches are being explored by Moletronics' investigators. For example, a group at the University of Notre

Dame, led by Marya Lieberman and Craig Lent, is developing a molecular-scale variant of the quantum cellular automaton (QCA) architectural approach[74] that relies on electric fields to communicate information through arrays of charged quantum dots, rather than currents traveling through wires. Not only could this approach radically reduce heat dissipation, but these edge-driven QCA systems have radically fewer interconnects to slow down processing when they must be charged and discharged. Prior to the beginning of the Moletronics Program, early demonstrations of QCAs were promising[75-77], but exploitation was slowed because of the difficulty in making a large number of solid-state quantum dots with the high degree of uniformity required. Also, using nearly micron-scale bulk solid quantum dots, QCA systems only operate at cryogenic temperatures, although the operating temperature rises exponentially as the size of the dot decreases. Molecules, with their very small sizes, extreme uniformity, and natural stability in the presence of excess charges seem to be natural structures to marry with the QCA approach. Thus, the Notre Dame group is developing molecules, like the one shown in Fig. 3c, to serve as pairs of quantum dots – i.e. quantum dot 'cells' – in a molecular QCA[78]. Under the auspices of the program, the Notre Dame investigators also are taking advantage of innovative biomolecular assembly techniques that work well for molecules to build arrays of such quantum dot cells[79].

Beyond this and other specific demonstrations of innovative architectural approaches, a council of computer architects has been established within the DARPA program. This council is considering ways that each of the experimental groups could optimize the performance of prototypes in any eventual larger-scale system demonstration. The architectural challenges associated with a large-scale molecular electronic computer system include[80,81] providing mechanisms for dissipating heat, execution fault tolerance (in addition to the above-mentioned tolerance against structural defects), mitigating crosstalk between closely-spaced wires, handling geometric and dynamic problems associated with the proliferation of interconnects in dense extended circuitry[82], as well as for harnessing as many as a trillion molecular devices to perform an efficient computation.

The immediate target of the Moletronics Program does not include a large-scale processor demonstration, however. Still, demonstrating logic circuits and large scale-memory arrays establishes the essential precursors for a molecular-scale electronic processor. Also, the circuitry actually demonstrated by the Moletronics Program may be used in the relatively near term to build hybrid molecular-silicon chips which improve upon the performance of more conventional silicon microprocessors.

Build, test, simulate...

Complementing experimental demonstrations in the Moletronics Program are efforts to build robust analytical models and simulation software tools to predict the behavior of molecular-scale devices, circuits, and the ultra-dense computing systems that soon will be built from them. There are two major molecular circuit and architecture simulation efforts underway. One, being conducted at Rice University, in collaboration with the Stanford Research Institute, is focused on analyzing and perfecting systems based upon the Rice-Yale-PSU random assembly strategy mentioned above. Another simulation development effort is being led by Seth Goldstein of Carnegie-Mellon University, who is collaborating with the MITRE Corporation to build a simulation tool called molecular SPICE or 'MolSPICE'. Initially, this effort is focused on simulating the molecular-scale crossbar circuits and systems first envisioned by the HP/UCLA team[53], and also adopted by Mallouk and Mayer's team at PSU, as well as by Goldstein and Budiu[83]. MolSPICE should have the potential for more general applicability, however.

Modeling and simulation are an essential part of the Moletronics Program for several reasons. First, at this stage of the technology, it is a time-consuming process to fabricate even small prototype molecular-scale logic circuits. Much time is absorbed in the trial and error of multiple attempts to get a working structure and organization for the system. It is anticipated that this time will increase as the prototype molecular-scale circuits and systems get larger and become more complex. Simulation is expected to provide a shortcut by testing the designs and their likely performance in software more quickly, before expensive experimental resources are committed to fabrication. For many years such modeling and simulation has played a large role in speeding product development in the microelectronics industry, and it is expected to have a similarly beneficial effect in moletronics.

Also, in the case of moletronics, some of the architectures being devised to take advantage of the unique properties of molecules are very innovative and experimental. It is critical

that novel architectural schemes be tested in advance to ensure that they scale up properly. This is especially true with respect to the more stringent requirements for defect tolerance in molecular electronic systems, as described above, since susceptibility to imperfections in manufacture can grow exponentially with the size of a system if appropriate measures are not taken to prevent this.

To ensure that Moletronics' systems are scalable in this way, a key element of the program's development strategy is that developers will build a little, test the molecular electronic system they have built, then simulate a still larger system from the test data, before building that larger system. This 'model-test-model' technique has been pioneered and applied with great success by DARPA for the development of other important information systems innovations.

The impending need to simulate large molecular circuit systems also is placing new demands upon analytic, theoretical models of the electrical behavior of molecules. While some of these can be quite accurate for small molecules, almost all take a huge amount of computer time and mass storage to solve the applicable quantum mechanical equations. For this reason, none of the analytic models are really satisfactory for modeling conduction in molecular systems of any appreciable size. Recognizing this gap in the present analysis capability, investigators at MITRE are attempting to develop simpler or faster quantum models for molecular circuits, as are Ratner at Northwestern University and Jorge Seminario of the Electrical Engineering Department at the University of South Carolina.

Already Seminario has applied such techniques to offer novel, easy-to-visualize explanations for the mechanism of operation of molecular diode switches[47-50]. Now, he is embarking upon a bottom-up strategy for providing detailed, but fast, quantum models for whole monomolecular circuits, starting with the switches and wires[84]. Some of these modeling efforts (e.g. Fig. 1c) are focused on providing details and insight into the dynamics at the interfaces between metal contacts and molecules, which often dominate the electrical behavior of circuits based upon small molecules[46]. Such modeling of the critical contacts may be refined via complementary experiments being led by Allara at PSU[44,45].

It is expected that, using such improved quantum models for molecular conductance, simulation systems such as the MolSPICE system will permit molecular electronics investigators to test their large scale architecture ideas before committing them to costly, time-consuming physical experiments.

Electronics beyond convention

A conventional view of the future of electronics, in accordance with the growth in density demanded by Moore's Law[80], suggests that sometime in the foreseeable future it will be necessary to carve up a centimeter-scale solid block of silicon into one trillion nanoscale pieces to make a computer processor. This would stretch materials science and technology up to or past the extreme physical limits of solid-state electronic materials[13]. The recent successes of the Moletronics Program and its investigators in demonstrating and applying new molecular-scale electronic materials show that it may not be necessary to go to such extremes in developing the present generation of materials. It has been shown that natural nanoscale molecular wires and switches function electrically with performance comparable to silicon, and that they can be made very cheaply chemically by the trillions of trillions. Also, they can be self-assembled via other inexpensive chemical processes into tiny operational computer logic and memory circuits.

Developments underway in the laboratories of Moletronics' investigators soon will expand both the extent and the variety of these molecular-scale electronic circuits and integrate them into ultradense computer systems. These prototypes of future systems show promise of not just maintaining Moore's Law, but of breaking it.

Looking beyond present experiments, it is possible to envision a new materials technology that incorporates such nanoelectronics into the very fabric of all objects even before they are built. Eventually, the same techniques that are being developed primarily for the fabrication of nanostructured electronics are likely to be applied more broadly to revolutionize the manufacture and the properties of all materials. MT

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