Technologies and Designs for Electronic Nanocomputers

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ABSTRACT

This paper reviews research developments aimed at the design of electronic computers that contain components with dimensions of only a few nanometers. A nanometer, one billionth of meter, is only about 10 atomic diameters. Such nanometer-scale electronic computers–i.e., electronic "nanocomputers"–that contain molecular-scale components are likely to be up to 10,000 times more densely integrated than today's smallest microcomputers. Electronic technology is one of several alternative technologies (e.g., mechanical, chemical, quantum) that have been proposed for implementing a nanocomputer. Electronic technology for nanometer-scale computers has the advantage, though, that it builds upon nearly a half century of experience and infrastructure developed for electronic computing. Electronic nanocomputers could be orders of magnitude faster than current electronic computers, as well as many times smaller or more densely integrated. Although some of the operating principles for electronic nanocomputers could be similar to present-day electronic microcomputers, there is a limit to how far the designs and fabrication technologies for present-day microcomputers can be scaled down. This has led some investigators to propose radically different "wireless" designs, quantum cellular automata, and nanometer-scale neural networks, all to be constructed from nanoscopic quantum-effect devices. These devices and designs take advantage of some of the very effects that have been obstacles to making smaller conventional transistors and circuits. Still other investigators have proposed the "self-assembly" of electronic devices with nanometer-scale components in order to circumvent some of the difficulties that have inhibited the fabrication of sub-micron structures using conventional lithographic techniques. This review examines critically a range of such technologies and designs for electronic nanocomputers. It describes and compares the operating principles, advantages, disadvantages, and status of the new technologies and designs that promise to continue the miniaturization of the electronic computer down to the scale of a few tens of nanometers and, ultimately, to the molecular scale. This information is presented in non-mathematical terms intended for a general, technically interested readership.

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I. INTRODUCTION

For the past forty years, electronic computers have grown more powerful as their basic subunit, the transistor, has shrunk [228]. However, the laws of quantum mechanics and the limitations of fabrication techniques soon will prevent further reduction in the minimum size of today's semiconductor transistors. Researchers have projected that once the smallest features of the transistor's design shrink to less than 0.1 micrometers (or microns, millionths of a meter), the devices no longer will function usefully [28,110,163–165,284]. In order to continue this miniaturization down to the molecular scale, present-day microelectronic device designs must be replaced with new designs that take advantage of the quantum mechanical effects that dominate on such a small scale.

There are a number of obstacles to making molecular-scale electronic computer devices. What will they "look" like? Upon what operating principles will they function? How will individual devices be connected together? Once designed, how will these computers be fabricated? This paper addresses these questions by reviewing the literature about ongoing research on the design of electronic computers integrated on the molecular scale. The authors have attempted to articulate a vision of future directions for the field based upon present developments. This vision and the answers to the questions above are presented in non-mathematical terms intended for a general, technically interested readership. However, this review article builds upon several, more technical and more specialized overviews [18,27,29,45,157,172,184,265,271,275,298,299] and treatises [55,244,306,312] that have preceded the present effort.

Molecular-scale electronic devices will measure less than 100 nanometers on a side. One nanometer (one billionth of a meter) is a linear distance spanning approximately ten atomic diameters. By way of comparison, the smallest features on today's commercially available, state-of-the-art integrated circuits have linear dimensions of about three hundred fifty nanometers (0.35 microns) [50,284]. If a transistor could be made with a 1 nanometer minimum feature size (the dimension of the smallest feature on a device), over 10,000 of such "nanodevices" would fit into the same area as a present day transistor. In other words, an electronic computer made of such nanometer-scale components–i.e., a "*nano*computer"–could be many orders of magnitude more powerful than today's *micro*computers.

Electronic nanocomputers could possess the advantages of high speed and low power consumption [88,128]. Such features would make them technically and economically desirable for a new range of applications [154]. This potential has been an enormous stimulus to research and development and has produced significant new advances at an increasing rate.

These advances have resulted from a synthesis of technical developments in diverse fields. Mathematical and computer modeling have shown that electronic nanodevices are possible [153,200,201,225–227]. In recent years, these new devices have been the subject of much speculation and research. Recent advances in the fields of physics [74], chemistry [83,267,302,315], molecular biology [140,294], and electrical engineering [57,271] have introduced tools and technologies of sufficient sensitivity [18,41,42,108,229,232,285] that the fabrication of prototype nanodevices has begun [7,46,53,74,92,251,268,269,272].

II. GENESIS OF NANOTECHNOLOGY

Scientific discussion of the development and fabrication of nanometer-scale devices began in 1959 with an influential lecture by the late, renowned physicist Richard Feynman [104]. Feynman observed that it is possible, in principle, to build and operate submicroscopic machinery. He proposed that large numbers of completely identical devices might be assembled by manipulating atoms one at a time. Feynman's proposal sparked an initial flurry of interest. However, it did not broadly capture the imagination of the technical community or the public [123]. At the time, building structures one atom at a time seemed out of reach.

Throughout the 1960s and 1970s advances in diverse fields prepared the scientific community for the first crude manipulations of nanometer-scale structures. The most obvious development was the continual miniaturization of digital electronic circuits, based primarily upon the invention of the transistor by Shockley, Brattain, and Bardeen in 1948 [138,159,252,253,282] and the invention of the integrated circuit by Noyce, Kilby, and others in the late 1950s [243,244]. In 1959, it was only possible to put one transistor on an integrated circuit [213]. Twenty years later, circuits with a few thousand transistors were commonplace [134,136,234,306].

This emerging trend in the miniaturization of transistors and the increase of their density in solid-state semiconductor circuitry was commented upon early by Gordon Moore, one of the founder's of the Intel Corporation. In the 1960s, Moore observed that the feature size for devices on a semiconductor chip was decreasing by a factor of 2 every 18 months. This empirical trend has continued and the principle has come to be called "Moore's Law" [244]. A timeline of key events in the development of nanotechnology is plotted in Figure 1 with Moore's Law for minimum feature sizes.

Developments in chemistry, molecular biology, and physics in the 1960s and 1970s were less obvious to the public than those in microelectronics, but were of equal technical importance. These advances continued to move towards manipulating matter atom by atom and molecule by molecule, rather than in bulk. The needs of the semi-

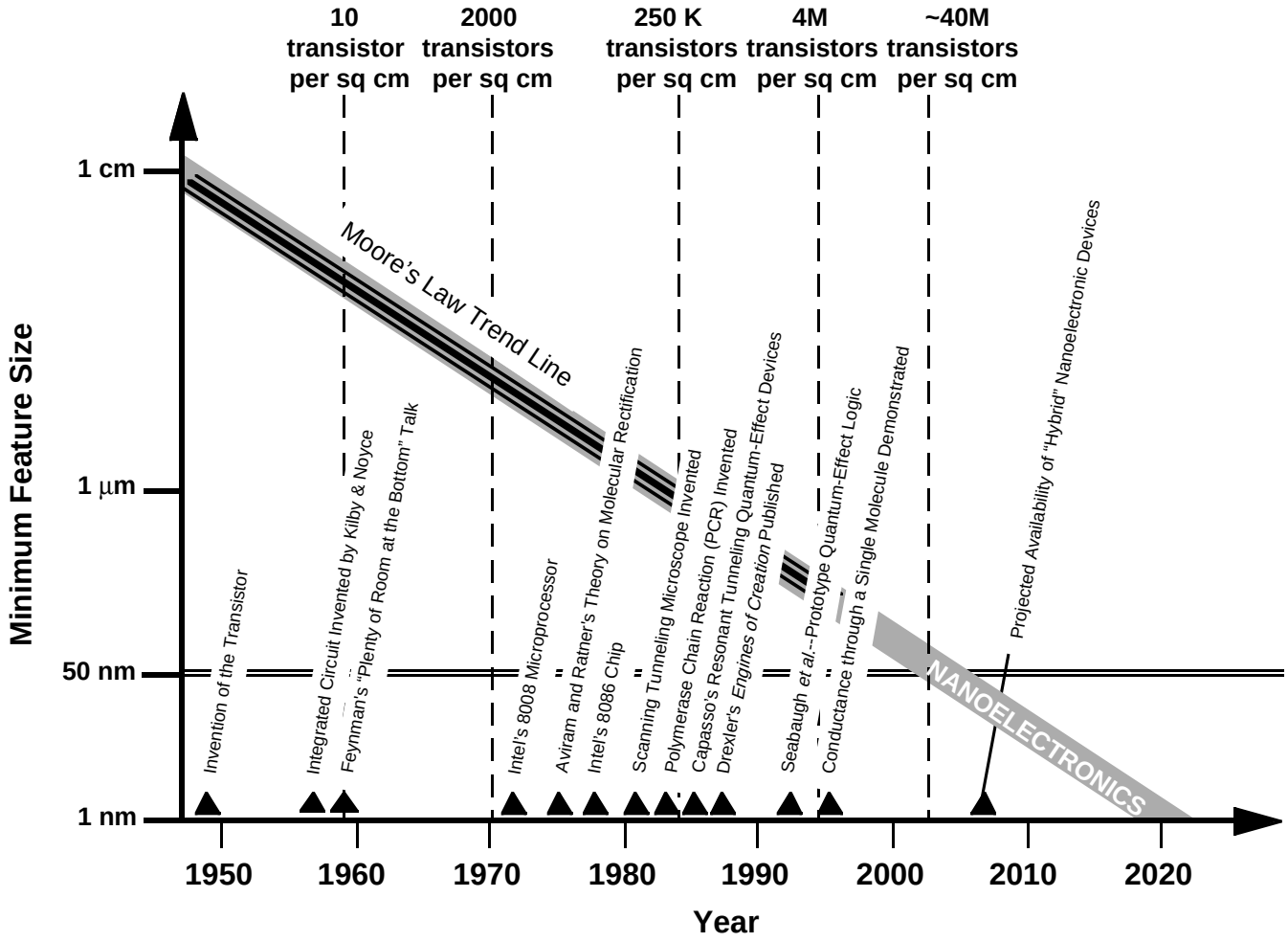

FIG. 1. Genesis of Nanotechnology. A timeline of selected key events plotted versus time with Moore's Law trend line.

conductor electronics industries, as well as those of a chemical and a petroleum industry stunned by boycott-induced shortages in raw materials, stimulated the adaptation of electron beams to characterize ever more precisely the nature of solid surfaces and the molecules that are adsorbed upon them [90,280,281]. Two farsighted scientists, Ari Aviram and Mark Ratner, began to envision electronic circuit elements made from *single molecules* and to show in detail how they would function [13].

In the late 1970s and early 1980s, biochemists and geneticists began using natural biological processes to build and manipulate proteins and other molecules [67,68,113,121,141,242]. They discovered how to splice short lengths of deoxyribonucleic acid (DNA) and ribonucleic acid (RNA) [73,76,99] into much longer sequences, leading to the development of the molecular genetics industry. In 1983, a biochemical process known as the Polymerase Chain Reaction (PCR) was discovered by Mullis [229]. With PCR, scientists were able to duplicate exponentially strands of DNA, amplifying a *few molecules* of genetic material into macroscopically measurable quantities [205].

Through the 1980s, the number of transistors that could be placed on a computer chip continued to increase exponentially. By the mid-1980s, one million transistors could be fit on a chip no more than 1 centimeter square [213]. Research also was progressing on advanced semiconductor materials that showed promise for high-speed electronics, such as gallium arsenide and silicon germanium [56,114,118,150,162,222]. Other research was examining the theoretical limits of computation and information processing [33–37,39,106,112,176,177]. Such fundamental physical considerations led to the conclusion that computers based upon conventional transistors had functional limits that soon would be approached [161,163–165]. A consensus began to build that the next-generation of electronic computers would be based upon much smaller devices in which quantum mechanical properties and the behavior of small numbers of electrons would be important [56,58,59,66,114,135].

In the 1980s, physicists were experimenting with many new quantum structures. They were capturing single electrons in potential wells termed "quantum dots" [91,94,158,248,249,287,306]. Quantum effects also were being harnessed in the development of scanning tunneling electron microscopes (STMs) and atomic force microscopes (AFMs) with which scientists could view and manipulate individual atoms [31,42,125,130,203,236,241]. These advances began lending credence to Feynman's vision of the creation and manipulation of molecular-scale structures and devices.

Scientists began using increasingly powerful computers to model and "design" the properties and structures of atoms, molecules, and solids, using an array of semi-classical and quantum-mechanical approximations [3,69,70,82,190,191,216,310]. Increasingly sophisticated and detailed computer graphics contributed greatly to the interpretative power and the physical insight provided by the refinement of computer-based, molecular-scale modeling approaches [82].

The combination of all these developments in diverse fields stimulated advances in the 1980s that put into place the rudiments of a true "nanotechnology." This term was invented by Taniguchi in 1974 [293], but it first was popularized in the 1980s by the scientist and visionary K. Eric Drexler in his book *Engines of Creation* [85]. Extrapolating from a scientific paper he published at the beginning of the decade [84], Drexler explained nanotechnology to a general audience. He described it as the knowledge and means for designing, fabricating, and employing molecular scale devices or "nanosystems" by the manipulation and placement of individual atoms and molecules with precision on the atomic-scale. Subsequently, *Nanosystems* became the title of a scientific treatise he wrote to justify in technical terms his vision of nanometer-scale machinery–computers, robots, and self-assembling systems [88]. Efforts to implement Drexler's ideas have served as one focal point for the new, interdisciplinary field.

In the 1990s, the convergence of developments in physics, chemistry, biochemistry, electrical engineering, and computer science are beginning to form a route toward a practical, useful nanotechnology. A revolution is occurring in miniaturization. The engineering and manufacture of micron-scale machinery has become an industry upon which further nanometer-scale miniaturization can be based [9,52,117,144,283,323,324]. Methods have become available for positioning single atoms [18,93,285], billions upon billions of copies are routinely made of a few identical molecules [205,230], and great strides are being made in the self-assembly of more complex structures from molecular building blocks [167,173,318]. Nanometer-scale quantum-effect devices, like "artificial atoms" or quantum dots, have been transformed from laboratory curiosities to the building blocks for future industries [157,158,271]. Molecular electronic devices such as molecular wires are no longer theoretical constructs. They have been synthesized [267] and demonstrated [53].

The computer and electronics industry is a particularly important focal point for this development. There, practical elements of nanotechnology–especially new techniques for nanofabrication [155,303,317,323,324]–are growing in importance as the semiconductor industry is approaching feature sizes of less than 100 nanometers and the physical limits of conventional, bulk-effect microelectronic devices [110,284]. Conventional microelectronic transistors are known to have lower bounds on their size. However, it is hoped that nanometer-scale replacements can continue the miniaturization of computational and information storage elements to the molecular level, with expectations for vast increases in memory density, power, and performance.

For these reasons, as well as the need for very small controllers to guide other micrometer-scale and nanometer-scale machinery, computers are at the top of the list of devices that the new "nanotechnologists" pro-

pose to build. However, there are a variety of opinions about the best way to design and build a nanocomputer. At least four distinct types of nanometer-scale computational mechanisms have been proposed: mechanical, chemical, quantum, and electronic [325].

A. Mechanical Nanocomputers

Drexler and his collaborators favor designs that resemble miniature Babbage engines, *mechanical* nanocomputers that would calculate using moving molecular-scale rods and rotating molecular-scale wheels, spinning on shafts and bearings [85,88]. Drexler also envisions that these would be assembled by the mechanical positioning of atoms or molecular building blocks one atom or molecule at a time, a process known as "mechanosynthesis." Once assembled, the mechanical nanocomputer would operate much like a vastly scaled down, complex, programmable version of the mechanical calculators that were familiar office tools in the period 1940 through 1970, preceding the introduction of widely available, inexpensive solid-state electronic calculators.

Strong arguments can be made in favor of such an approach [86–89,128]. For one thing, quantum mechanics assures that the molecular-scale moving parts should not be subject to the large frictional effects that defeated earlier attempts to build complex macroscopic mechanical computers, such as those designed by Charles Babbage in the 1830s and 1840s. However, there are near-term drawbacks. One such drawback is that the fabrication of such nanomechanical devices is likely to require "hand-made" parts assembled one atom or molecular subunit at a time using STMs in processes that are relatively slow. While this might be done, it would be tedious work to move even a few atoms into a specific position this way, and it would be increasingly more difficult to manufacture reliably the many precision parts for the computer. It is possible, though, that this problem might be alleviated, somewhat, by the perfection and evolution of recently developed micro-STMs that could be constructed in arrays to build many nanometer-scale components in parallel [323,324]. Stereospecific chemical reactions and chemical self-assembly also might be applied to help realize a mechanical nanocomputer. Beyond the problem of fabrication, many other practical issues must be addressed, such as how to power and program nanomachinery.

Drexler's work has argued strongly for the *theoretical* possibility of building nanomechanical computers. The engineering of such devices lags somewhat behind that of other proposed approaches, though. The authors believe the engineering of nanomechanical computers would be advanced greatly by more specific proposals for the design and step-by-step fabrication of a simple nanomechanical logic device, say a four-bit machine that uses a variant of Drexler's rod logic [87].

B. Chemical Nanocomputers

In general terms, a *chemical* computer is one that processes information by making and breaking chemical bonds, and it stores logic states or information in the resulting chemical (i.e., molecular) structures. A chemical *nanocomputer* would perform such operations selectively among molecules taken just a few at a time in volumes only a few nanometers on a side. Proponents of a variant of chemical nanocomputers, *biochemically* based computers, can point to an "existence proof" for them in the commonplace activities of humans and other animals with multicellular nervous systems [139,140]. Nonetheless, artificial fabrication or implementation of this category of "natural" biochemically based computers seems far off because the mechanisms for animal brains and nervous systems still are poorly understood. Very recently, however, Adleman has taken a giant step towards a different kind of chemical or artificial biochemical computer [1,26,169]. He used fragments of DNA to compute the solution to a complex graph theory problem.

Adleman's method utilizes sequences of DNA's molecular subunits to represent vertices of a network or "graph". Thus, combinations of these sequences formed randomly by the massively parallel action of biochemical reactions in test tubes described random paths through the graph. Using the tools of biochemistry, Adleman was able to extract the correct answer to the graph theory problem out of the many random paths represented by the product DNA strands. Like a computer with many processors, this type of DNA computer is able to consider many solutions to a problem simultaneously. Moreover, the DNA strands employed in such a calculation (approximately 10^{17}) are many orders of magnitude greater in number and more densely packed than the processors in today's most massively parallel electronic supercomputer. As a result of the Adleman work, the chemical nanocomputer is the only one of the aforementioned four types to have been demonstrated for an actual calculation.

It seemed at first that Adleman's method would be limited to the solution of combinatorial problems. More recent work by Lipton and by Lipton and his collaborators has shown, though, how the approach may be applied to a much wider class of digital computations [48,196]. Nonetheless, the issue of fast, efficient input and output, techniques to reduce or compensate for error, and a number of other obstacles remain to be addressed to permit this promising new approach to be applied commonly to computational problems.

There are other proposals, as well, to use biochemicals in computing. For example, Birge has suggested the use of the protein dye bacteriorhodopsin that is produced by some bacteria. He and his collaborators have shown that it could provide a very high density optical memory that could be integrated into an electronic computer to yield a hybrid device of much greater power

than a conventional, purely electronic computer [44,129]. Nadrian Seeman also has proposed alternative ways to use branched DNA for the nanometer-scale assembly of molecular electronic devices [273].

C. Quantum Nanocomputers

Recently, there has been serious interest in the possibility of fabricating and applying nanometer-scale *quantum* computers [38,81,133,197,199,278]. In a quantum computer, it is proposed that massively parallel computations can be performed through the "natural" mechanism of interference among the quantum waves associated with the nanometer-scale components of a multicomponent, coherent quantum state. Proposed quantum computers would represent each bit of information as a quantum state of some component of the computer, e.g., the spin orientation of an atom. According to quantum mechanics, the state of each nanometer-scale component of a system can be represented by a wave [11,12,19,81,105,122,221]. These quantum matter waves are analogous to light waves, except that their wavelengths tend to be much shorter, in inverse proportion to the momentum of the quantized component. Thus, the quantum waves might be manipulated in the space of only a few nanometers, unlike most light of moderate, nondestructive energy, which has wavelengths of several hundred nanometers.

By carefully setting up the states for the components of the quantum system, a desired computation could be performed through the wave interference among the quantized components. All discrete computational paths would be considered at once, at the speed of light, through the wave interference patterns–fast, intrinsic parallel computation. Given the correct initial preparation of the entire multicomponent computational system, constructive interference among the components' waves would emphasize those wave patterns which correspond to correct solutions to the problem, and destructive interference would weed out the incorrect solutions.

The idea for a quantum computer is based upon the work of Paul Benioff [33,34] in the early 1980s and that of David Deutsch [78] and Richard Feynman [106,107], in the mid-1980s. Although quantum computers originally were proposed as a theoretical construct for considering the limits of computation [33], some researchers have suggested that fundamentally hard and economically important problems could be solved much more rapidly using quantum interference and parallelism [78]. In particular, Shor has proven that a quantum computer could factor large numbers very rapidly and thereby, perhaps, provide cryptographers with a powerful new tool with which to crack difficult codes [278].

Some proposals have been made for implementing such a computer [38,65,72,197]. Lloyd, in particular, has attracted much attention recently with a mechanism he has proposed for the practical implementation of quantum computers [198,199]. There have been some quantitative arguments, though, that cast doubts upon the specifics and the ultimate utility of Lloyd's proposals [206]. More general reservations about proposed quantum computers include the fact that they would have to be assembled and initialized with great and unprecedented precision. Quantum computers would be very sensitive to extremely small physical distortions and stray photons, which would cause the loss of the phase coherence in the multicomponent quantum state. Thus, they would have to be carefully isolated from all external effects and operated at temperatures very close to absolute zero. Even then, errors are likely to remain an intrinsic feature of the quantum computational mechanism as they are in the stochastic mechanism of the DNA biochemical computers discussed above. Fault-tolerant architectures could compensate for this difficulty. Thus, error alone does not rule out the eventual design and application of quantum computers for solving certain classes of difficult problems. Much scientific effort is being devoted to that goal, and several intriguing new designs for implementing quantum computers have been proposed recently [72,292].

Quantum computation also is likely to benefit from advances in other, related fields. For example, experiments with microelectromechanical systems and quantum dot lasers are reducing the size of coherent radiation sources. Such developments are likely to reduce the size of the bulky apparatus that now is necessary for experiments with quantum computers and permit these devices to evolve toward dense nanometer-scale integration.

D. Electronic Nanocomputers

Because of 50 years of experience worldwide with electronic digital computers, including the extensive research and industrial infrastructure built up since the late 1940s, *electronic* nanocomputers appear to present the easiest and most likely direction in which to continue computer development in the near future. The power and speed of computers have grown rapidly because of rapid progress in solid-state electronics dating back to the invention of the transistor in 1948 [213,234]. Most important, there has been exponential increase in the density of transistors on integrated-circuit computer chips over the past 40 years [165]. In that time span, though, there has been no fundamental change in the operating principles of the transistor. Even microelectronic transistors no more than a few microns (millionths of a meter) in size are bulk-effect devices. They still operate using small electric fields imposed by tiny charged metal plates to control the mass action of many millions of electrons [240,259].

At the current rate of miniaturization, the conventional transistor technology will reach a minimum size limit at the turn of the century. At that point, small-scale quantum mechanical effects, such as the tunneling

of electrons through barriers made from matter or electric fields, will begin to dominate the essential effects that permit a mass-action semiconductor device to operate [271]. Nonetheless, to maintain the current rate of advance in computer speed and information storage capacity, there must be continued increases in the density of computational elements on integrated circuit chips. This seems to mandate continued decreases in size for the transistor. Thus, it is evident that a change in the technology of the transistor will be necessary.

Still, an electronic nanocomputer will continue to represent information in the storage and movement of electrons. To perform these functions on ever smaller scales a range of device technologies have been proposed to modify or replace the conventional microelectronic transistor. There are single-electron transistors that are in many ways similar to today's microelectronic transistors, especially in their switching and amplification processes [157,192]. Although these devices operate by the movement of *single* electrons, they are not "quantum-effect" devices because they have high resistances intentionally designed to destroy quantum interference effects among the many electrons that occupy the volume of the device [193].

However, many of the devices that are the most widely investigated and discussed as nanometer-scale replacements for the transistor do employ quantum interference and tunneling–i.e., some of the same quantum effects that prevent much further shrinkage or "scaling" of bulk-effect transistors [27]. Quantum dots (or "artificial atoms") govern tunneling of a small number of electrons through the influence of an electric field from a nearby gate electrode [158,248,249,306]. Present-day quantum dots can be made as small as 30 nanometers [231,290]. In the future, they are likely to be made even smaller. Also, the quantum dot devices are sensitive to and can take advantage of the presence or absence of the charges of single electrons. Other electronic nanodevices that take advantage of quantum mechanical effects, such as resonant-tunneling devices, also have been proposed, fabricated, and used in experiments [57,110,271].

Still smaller *molecular-scale* electronic devices may be possible [140,232]. One of the first examples of a specific proposal for a molecular-scale electronic device was a rectifier proposed by Aviram and Ratner in 1974 [13]. The rectifier consisted of a single molecule that would demonstrate almost ideal diode characteristics in passing current preferentially in one direction. More recently, a molecular shift register that operates based on electron transfer has been proposed [142,311], a Japanese group has simulated atomic-scale switches [309], and a molecular "shuttle" switch has been synthesized [46]. Also, Drexler and Merkle have suggested a more radical construct that they term helical logic to be based upon the helical, atomic-scale motions of electrons in an applied, rotating electric field [217].

There are a wealth of still other proposals and research on ways to scale down and extend electronic computing into the nanocosm. Thus, while nanocomputers using one of the alternative operating principles described above (mechanical, chemical, quantum) ultimately may prove superior, the authors believe that in the near term, at least, smaller electronic computers are likely make the best use of the infrastructure developed by almost fifty years of experience with larger electronic digital computers. For that reason, the rest of this paper will focus on technologies and designs for building electronic nanocomputers.

III. CURRENT COMPUTER TECHNOLOGY: MICROELECTRONIC TWO-STATE DEVICES

Before examining designs for electronic *nano*computers, it is important to understand how current electronic *micro*computers function [165,211,240,259,288]. Imagine taking a computer apart and successively peeling away layers of its construction. At the highest level, a computer can be separated into two parts: a memory and a central processing unit (CPU). An ideal computer is a machine that is set up with inputs and uses the rules of Boolean logic to transform them into outputs [128]. The CPU is the part of the computer that does the logical transformations. It is made up of a large number of electronic logic gates–e.g., AND, OR, NOT. Each of these logic gates is actually a circuit made up of several transistors. Indeed, the transistor is the building block for most devices in an electronic computer. Current microprocessor chips, such as Intel's Pentium chip, contain over 3.2 million transistors [188].

In digital circuits, the transistor is usually used as a two-state device, or switch. A transistor can be either "on" or "off," with a rather large difference between the two states. The state of a transistor can be used to set the voltage on a wire to be either high or low, representing a binary 1 or 0 in the computer. By building different circuits containing transistors as two-state devices, any boolean logic function can be implemented.

The transistor's second function in a computer is that of an amplifier. A transistor is able to take a small input signal, and output a new signal that is many times larger than the original signal. Amplification allows signals to be transmitted through switches inside the computer without a loss of strength [165].

The metal-oxide-semiconductor field effect transistor (MOSFET) has been by far the most common type of transistor in modern digital circuits, since Shockley's explanation of the device in 1952 [137,136]. MOSFET circuits use very little power and are economical to fabricate. As shown in Figure 2, the field effect transistor has three terminals which are usually called the source, the drain, and the gate. The MOSFET controls the flow of current from the drain to the source by changing the voltage on the gate [244]. If the voltage on the gate of the transistor is zero, very little current will be able to flow from the drain to the source of the transistor. However,

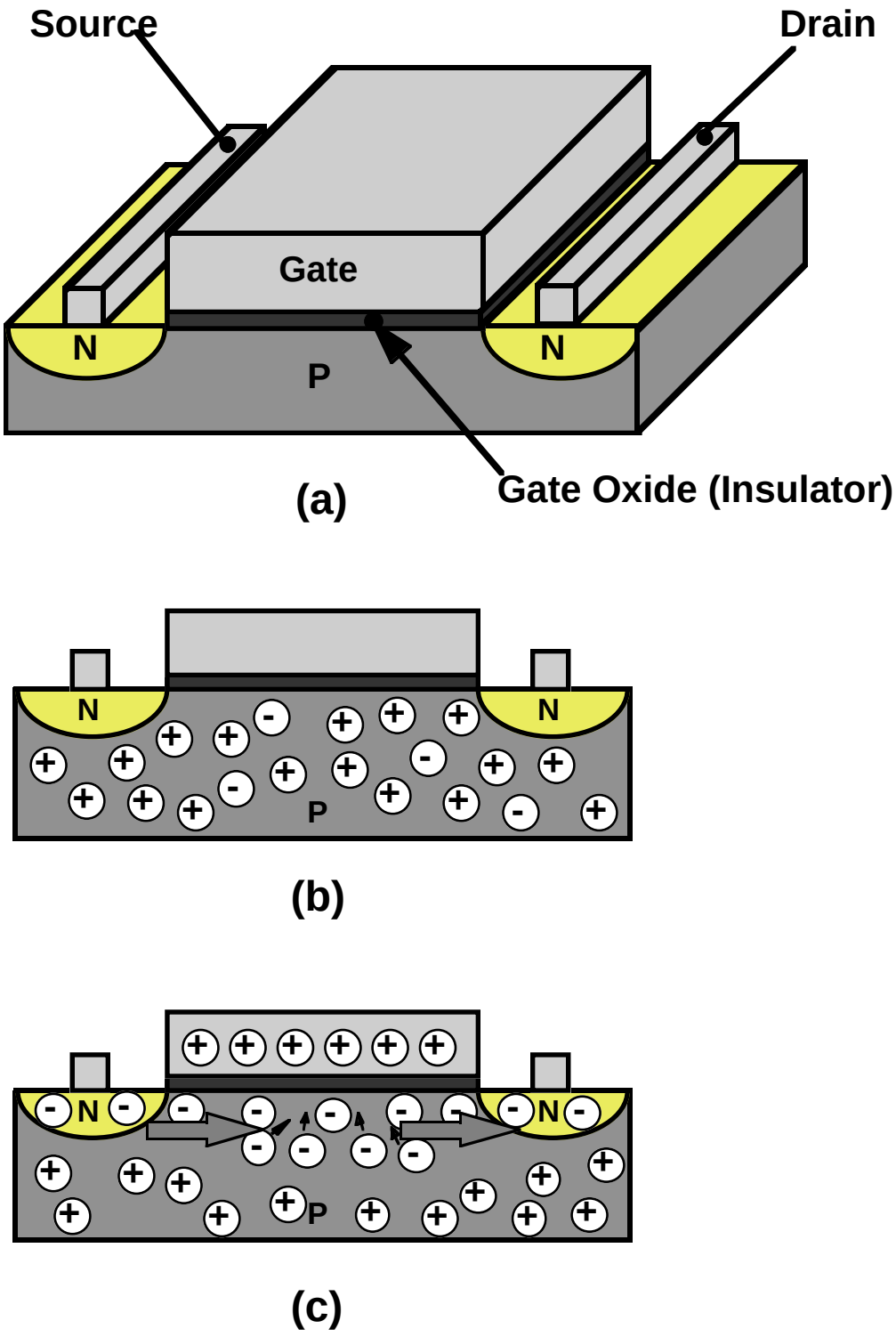

FIG. 2. Cross-Section of a NMOS Transistor. The transistor shown in the schematic cross-section in (a) is the basic building block of microcomputers. When there is no voltage applied to the gate electrode as in (b), no current can flow through the semiconductor. However, when voltage is applied to the gate electrode in (c), the electrons (negative circles) segregate from the holes (positive circles) to form a "channel" which permits current (large white hatched arrows) to flow between the source and the drain.

if the voltage on the gate of the transistor is increased, the current that can flow between the other two terminals will be increased greatly. This distinct change in conductivity gives the MOSFET the properties of a two-state device. Also, since small changes of gate voltage result in large changes in conductivity, the MOSFET can be used as an amplifier.

A. How a MOSFET Works

Besides using very little power and being easy to fabricate, the MOSFETs ability to be scaled down is a major reason why the design has continued to be so pervasive. In the past, the most common way to make smaller electronic circuits has been simply to shrink the dimensions of all of the circuit components by a constant factor. This process is called "scaling." The MOSFET has remained popular because its operation changes very little as it is scaled down to much smaller sizes. As MOSFETs reach minimum feature sizes of 100 nanometers, it is not clear that this will still be true. There are physical reasons why field effect transistors will not be useful as truly nanometer-scale switching devices. In order to understand the physical limits of scaling, one must first understand the physics behind the operation of the MOSFET [240,244,259].

The name "metal-oxide-semiconductor field effect transistor" is derived from the materials that the transistor is made from. MOSFETs are built upon a substrate of doped silicon. Dopants are materials, such as boron or arsenic, that are introduced into the silicon to create an excess or surplus of valence electrons. Negatively doped (N-doped) silicon contains free electrons that are able to move through the semiconductor. Positively doped (P-doped) silicon contains electron vacancies, commonly known as "holes," which can be thought of as positive charges that are also free to move through the material.

The most common type of MOSFET is the NMOS transistor. NMOS refers to the way the different parts of the transistor are doped. NMOS transistors consist of two N-doped regions of silicon that are slightly separated on a P-doped substrate [137]. This arrangement is illustrated schematically in Figure 2(a). The two N-doped regions are the source and drain of the transistor. An oxide barrier is placed over the region between the source and the drain. Metal contacts are attached to the source, drain, and the oxide barrier. The connection to the oxide barrier serves as the gate of the MOSFET.

The P-doped region shown in Figure 2(a) between the source and the drain is called the "channel." It is given this name because when the device is "on" electrons travel through the channel on the way from the source to the drain. The channel is separated from the gate by the insulating oxide barrier. When the voltage of the gate is below a certain threshold voltage, very few electrons can pass from the N-doped source through the P-doped channel as illustrated in Figure 2(b). However, when the gate voltage is increased, the positively charged holes in the channel are repelled away from the oxide barrier, and electrons are attracted to it. This shift of negative charge towards the oxide barrier creates a thin N-doped layer in the channel. With this N-doped channel in place, current can easily flow from the source to the drain. This is illustrated in Figure 2(c). Thought of in another way, the electric field induced by the charge on the gate causes the charge in the channel to shift, increasing its conductivity. This is the reason why the device is called a "field effect" transistor.

B. Obstacles to the Functioning of Nanometer-Scale Transistors: Limitations to Scaling

Scaling down the MOSFET design has worked well up to current commercial device sizes, but when MOSFETs are fabricated below 100 nanometers in size, certain factors may inhibit their usefulness [163–165,213,274,284]. One hundred nanometers, or 0.1 micron, is often called the "0.1 micron barrier." Beyond this barrier, many scientists believe that new devices will need to take the place of the MOSFET. Several of the effects that limit the MOSFETs scalability are discussed in this section of the paper.

1. Shrinkage of Depletion Regions

Near the interface between a N-doped and a P-doped region of silicon, the free electrons and holes recombine to form a region that is depleted of charge carriers. This depletion region restricts current from flowing across the interface. In a MOSFET, depletion regions form the barrier that prevents current from flowing between the source and drain when the transistor is off. As depletion regions are squeezed down to a thickness less than 0.1 microns, their ability to block current is impaired [110]. Transistors smaller than 0.1 microns must use a different mechanism in order to control the flow of current through the device.

2. High Electric Fields

In order for a signal in a circuit to be recognizable, it needs to be distinguishable from thermal noise. Thus, the random voltages caused by thermal noise serve as a lower bound for some of the operating voltages of the MOSFET. As the field effect transistor is shrunk, this voltage is applied over a much shorter distance, increasing the electric field inbetween. As electric fields become higher, electrons achieve higher kinetic energies traveling from the source to the drain. Once these electrons reach a high enough kinetic energy, they can knock free other

electrons in the solid, stimulating an uncontrollable surge of current in the transistor, or "avalanche breakdown." This prevents the device from operating properly. The threshold for avalanche breakdown sets a maximum electric field that can exist in a MOSFET [164,165].

High electric fields also cause another problem in field effect transistors. At high energies, a few electrons are able to travel into the insulating barrier and become trapped. One of the purposes of the insulating barrier is to prevent current from flowing from the gate to the rest of the transistor. According to Keyes [164], it is rare for electrons to enter the oxide barrier, but they accumulate over time, ruining the operation of the device.

3. Tunneling

Transistors are separated from each other on integrated circuits so that the operation of one does not affect the operation of the others. The insulating material inbetween adjacent transistors can be thought of as a potential energy barrier.

According to classical physics, if the total energy of an electron in a transistor is less than the energy of the potential barrier, then it can not pass through the barrier to a neighboring transistor. According to the laws of quantum mechanics, however, if the barrier thickness is small enough, there is a significant probability that the particle will be able to cross the barrier even if its energy is less than the energy of the barrier [12,19,102,105,122]. This process is called "tunneling," and it limits the functional density of MOSFETs. Tunneling increases exponentially as the barrier thickness is decreased. Tunneling also increases if the height of the potential barrier is lowered.

The insulating barriers between transistors are large enough to prevent such tunneling, but the oxide barrier between the gate and channel is not. With further miniaturization of the transistor, the oxide barrier would become thin enough that electrons would begin to tunnel through. At this point, the distinction between on and off in the transistor would disappear. However, distances need to shrink to approximately 2.5 nanometers before considerable tunneling through the gate oxide occurs [193].

4. Heat Dissipation

The amount of heat that is dissipated per square centimeter on integrated circuits has been increasing steadily as devices and circuitry have become smaller and more densely spaced. The amount of heat given off by many chips far exceeds that of most cooking surfaces. Were it not for cooling mechanisms, the chips would melt themselves down. Hall has pointed out that if this trend were to continue down to the molecular scale, nanocomputers would give off as much heat per unit volume as gunpowder! [128] Conventional integrated circuit designs eventually will be limited in density by the amount of heat that they dissipate [160,166].

Proposals to limit heat dissipation in computers often focus on the idea of making the computational process thermodynamically reversible, or more nearly so [35,37,112,128,220]. However, a thermodynamically reversible process for a computer that consists of a large number of computational elements necessarily is a slow process. Also, because error correction is a dissipative process, a reversible computing process tends to accumulate in the output a large number of errors produced by noise in the computer system or its surroundings. As computing elements are made smaller and more densely packed, heat dissipation per element must be reduced. It is likely, however, that this requirement will have to be balanced against the requirements to maintain sufficient computational speed and resistance to errors. Maintaining this balance would impose limits on the possibilities for reducing heat dissipation.

5. Vanishing Bulk Properties

Most MOSFETs are made of regions of silicon that are doped with impurities. The ratio of impurity to silicon typically is very low. When transistors are made below 100 nanometers in size, dopant atoms may number only in the tens or hundreds. The relatively massive flows of electrons and holes that allow modern transistors to function will not longer be possible in devices this small. Moreover, the placement or distribution of the few dopant atoms will vary, statistically, and this variation is likely to cause extreme differences in the operation of similar devices [309]. These obstacles to scaling illustrate the dependency of the MOSFET on bulk properties of semiconductors.

Once electronic devices approach the molecular scale, the bulk properties of solids are replaced by the quantum mechanical properties of a relatively few atoms. Properties associated with doped semiconductors will become less evident and influential in the operation of an electronic device. Quantum mechanical effects, such as energy quantization and tunneling become much more significant. In order for a transistor to work on the molecular scale, it must operate based on these effects, rather than in spite of them [27].

IV. FUTURE TECHNOLOGIES: LIKELY APPROACHES TO NANOELECTRONIC TWO-STATE DEVICES

A number of nanometer-scale replacements for the bulk-effect semiconductor transistor have been suggested to overcome the difficulties discussed above. This section

will present several of these devices that show potential as nanoelectronic two-state devices. Several questions about each device will be answered, as follows:

- How does (or would) the device function?
- What would be its advantages and disadvantages?
- At what stage of development is the device?

All of these devices function based upon the principles of quantum mechanics [11,12,19,102,105,122,221]. However, the overall speed of each device depends on the manner in which they apply and take advantage of these principles. The sizes of the various devices also vary. These properties, as well as other merits unique to each device, will be discussed. Some of these devices, such as resonant-tunneling transistors and single-electron transistors, already have been fabricated in the laboratory. Others, such as molecular relays, are only in the modeling stage. The stage of development of each device also will be addressed. The information of this type from the following sections is summarized in Table I.

A. Resonant-Tunneling Transistor

Resonant-tunneling devices (RTDs) are one possible option for making nanometer-scale two-state devices. Many RTDs already have been fabricated and tested [271]. RTDs usually are constructed from semiconductor heterostructures made from pairs of different III/V alloys, such as the pair GaAs and AlAs [114,312]. As depicted in Figure 3(a), a resonant-tunneling diode is made by placing two insulating barriers in a semiconductor, creating an island between the two insulators [57]. Resonant-tunneling diodes can be made with center islands approximately 10 nanometers in width. Whenever electrons are confined between two such closely spaced barriers in this way, the quantum wave properties of the electrons restrict their energies to certain discrete levels or to energy bands consisting of groups of discrete levels closely spaced in energy [12,19,27,102,122]. Only a finite, integral number of discrete, "quantized" energy levels can exist inside the potential well. This energy quantization is the basis for the operational mechanism of the resonant-tunneling diode.

The only way for electrons to pass through the device is to tunnel through the two barriers. The probability that the electrons can tunnel is dependent on the energy of the incoming electrons compared to the internal energy levels of the device. As illustrated in Figure 3(b), if the average energy of the incoming electrons differs from the energy levels allowed inside the potential well, current does not flow. However, when the average energy of the incoming electrons aligns with one of the internal energy levels as shown in Figure 3(c), current flows through the device. When current flows through the device, the energy level of the electrons outside the well is said to be in "resonance" with the energy level of the electrons inside the well. These resonances correspond with sharp peaks in the plot of current versus voltage (energy of the incoming electrons) for the diode, as illustrated in Figure 4 [57].

RTDs have been incorporated into conventional bipolar junction transistors (BJTs) [244]. A bipolar transistor is a three terminal device similar to the MOSFET. However, instead of being a voltage-controlled amplifier as is a MOSFET, a BJT is a *current*-controlled amplifier. The three terminals of the BJT, called the base, emitter, and collector, are analogous to the gate, source, and drain of a MOSFET, respectively. The current flowing into the base (gate-analog) affects the amount of current that flows between the emitter and collector. Since small changes in the base current are multiplied into large change in collector current, the BJT can be used as an amplifier.

By building an RTD into the emitter of a BJT, a "resonant-tunneling transistor" can be made. In this compound or "hybrid" nanoelectronic-microelectronic device, the RTD serves as a filter that only allows current to flow into the emitter of the BJT at certain base-emitter voltages. These voltages correspond to internal energy levels of the RTD. At low base-emitter voltages, no current can flow through the base-emitter RTD so the transistor is "off." As the base-emitter voltage is increased to coincide with the first internal energy level of the RTD, the base current can pass through the RTD, and the transistor is "on." Used in this way, a resonant-tunneling transistor is a two-state device. However, because the RTDs at the emitter can be designed with any number of conductance peaks, the transistors can have multiple "on" states and multiple "off" states. A schematic of a resonance tunneling transistor is depicted in Figure 5.

Multistate transistors can reduce the number of devices necessary to implement logic functions, and therefore, increase the density of logic in integrated circuits [223,272]. Frazier, Seabaugh, and others at Texas Instruments have constructed such devices and demonstrated their operation at high temperature [268–271,289]. The progress at Texas Instruments is based upon earlier work on the resonant-tunneling transistor by Capasso and his collaborators at AT&T Bell Laboratories. The particular scientific and engineering merit of this "hybrid" micrometer-scale/nanometer-scale technology is that it builds explicitly upon the principles and existing infrastructure of microelectronics to "bootstrap" the leading edge of technology into the useful application of nanometer-scale quantum-effect devices. Hybrid nanoelectronic-microelectronic devices could accelerate the arrival of the "nanoelectronic era" of widely available digital logic based on quantum-effect nanometer-scale devices. This is illustrated in Figure 6.

Nonetheless, since nanometer-scale resonant-tunneling transistors are built into conventional bipolar transistors to make a resonant-tunneling transistor, the size of the overall hybrid device still is limited by the scaling prob-

Device	Operating Principle	Status	Advantages	Disadvantages
Resonant Tunneling Transistor	Quantum resonance in double barrier potential wells	Capable of large scale fabrication	Logic compression Semiconductor based	Limits on scaling similar to microelectronics
Single Electron Transistor	Coulomb blockade	Experimental; only operates at very low temperatures	High gain Operation principles similar to MOSFET	Low temperature Difficult to control
Quantum Dot Cell	Single electron confinement in arrays of quantum dots	Quantum dots can be fabricated; quantum dot cells are still theoretical	Wireless Low energy dissipation	Difficult design rules Susceptible to noise
Molecular Shuttle Switch	Movement of a molecular "bead" between two stations on a molecule	Experimental, can only be switched chemically	Small but robust Assembled chemically	Slow switching speed How to interconnect?
Atom Relay	Vibrational movement of a single atom in and out of an atom wire	Theoretical	Very high speed Subnanometer size	Low temperature Very unreliable
Refined Molecular Relay	Rotational movement of a group in and out of an atom wire	Theoretical	Subnanometer size More reliable than atom relay	How to fabricate? How to interconnect?

TABLE I. Summary of Nanoelectronic Two-State Devices

Design	Operating Principle	Status	Advantages	Disadvantages
Traditional Wired Design	Switching devices are connected with metal or doped polysilicon wires	Design has been used in microelectronic computers since the invention of the integrated circuit	Fabrication tolerances do not have to be atomically precise Not as susceptible to noise	Sub-micron wires have short lifetimes ($<$ 100 hours) Sub-micron wires have high resistance, so they are slow
Wireless Ground State Computing (QCAs)	Insulated quantum dots influence each other with electrostatic fields. The computer is driven towards the ground state of the system of electrons	Theoretical	Interconnection speed is extremely fast, and can work on the nanometer scale Very low power dissipation	Total system relaxation time is slow Design rules are complicated
Wireless Dissipative Computing	Insulated quantum dots influence each other with electrostatic fields. Computation is done with metastable states.	Theoretical	Fast interconnects Simple design rules	Sensitive to background charge Can all circuits be implemented?
Nanometer-scale Nonlinear Networks (NNNs)	Array of interconnected devices. Analog computing with synaptic laws	Theoretical	Primarily local interactions Use nonlinearities in charge transport	Sensitive to stray charges

TABLE II. Summary of Nanocomputer Logic Designs

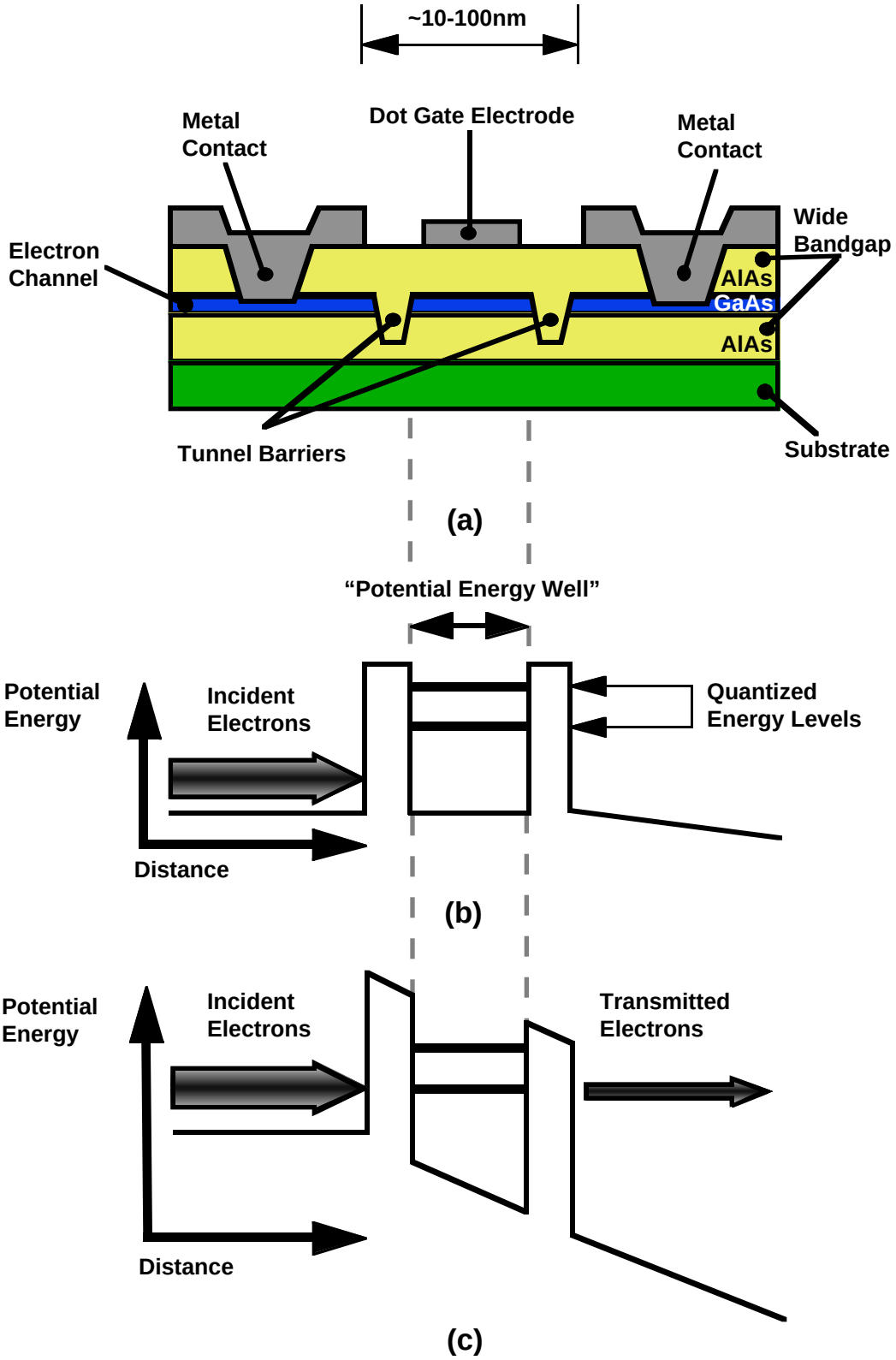

FIG. 3. Schematic of a Resonant-Tunneling Diode (RTD). The physical structure of the RTD in (a) maps to the potential energy diagram in (b). The AlAs barriers create the potential energy barriers that define the size of the potential well. The depth of the well is controlled by the dot gate electrode. By lowering the potential of the well and applying a constant potential across the RTD ("downhill" slope) in (c), the energy of the incident electrons is aligned with the allowed energy levels inside the well, allowing current to flow through the device.

lems associated with *micro*electronic bulk-effect devices. However, there is the strong possibility that purely nanometer-scale devices based upon resonant tunneling also will be developed [245,246].

B. Single-Electron Transistor

Single-electron devices, such as single-electron transistors [157,192], capture or release single electrons or holes within a sea of background electrons (on the order of 10^7). Such devices are not electrostatically isolated from their surroundings. Therefore, their operation is *not* dominated by quantum effects like the interference among a few electrons. Rather, the operation of an SET depends on the movement of a single electron due to its electrostatic interaction with the large number of other surrounding electrons [193].

A schematic of an SET is shown in Figure 7. The electron "island" in an SET is so small that it can hold only a few free electrons. [62,66,79,116,157,158,192,286]. Electrons can tunnel onto the island one at a time from a nearby wire, the source, and then off the island onto another nearby wire, the drain. This produces a measurable flow of current. However, since the island can only be occupied by a few electrons, extra electrons generally are prevented from tunneling onto the island by the electrostatic repulsion of those already occupying the island, and thus, no current flows. This opposition to tunneling is called "Coulomb blockade."

In order to control the number of electrons on the island, a metal gate electrode is introduced nearby. A sufficient increase in the voltage of the gate electrode will induce an additional electron to tunnel onto the island from the source. The extra electron soon tunnels off onto the drain. This double-tunneling process repeats millions of times a second, creating a measurable current through the island. Since the current between the source and drain is sensitive to the charge of single electrons on the gate, the amplification ratio, or "gain," can be extremely high.

As the gate voltage is increased further, the number of electrons on the island stabilizes at a value one higher than before, and again no current flows. Yet further increases in gate voltage cause more electrons to migrate on the island, and each increase of one electron is heralded by a spike in current flow.

At high temperatures, however, the thermal energy of electrons in the surrounding medium may overcome the Coulomb blockade, allowing electrons to tunnel onto the island and current to flow under all gate voltage conditions. Thus far, the low temperatures needed to preserve the SET's ability to switch current on or off have been a major obstacle to their practical application. However, sufficiently small SETs would work even at room temperature. A group at NTT in Japan has succeeded in making such an SET only 30 nanometers across. It exhibits Coulomb blockade at 150 degrees Kelvin [231,290]. This is well above the boiling temperature of liquid nitrogen, 77 degrees Kelvin. This development eventually could lead to more routine use of SETs, and even, possibly, their eventual operation at room temperature (300 degrees Kelvin).

C. Electrostatic Quantum Dot Cells

"Quantum dots" are small potential wells or "boxes" that electrostatically isolate a single electron or a few electrons from their surrounding environment [21,22,24,181,182]. The number of electrons in a dot can be adjusted by changing the electrostatic environment of the dot. Presently, quantum dots are constructed with tiny insulated regions of conducting material ranging from 30 to 100 nm in size, and holding from zero to hundreds of electrons. Figure 8 illustrates the concept of a quantum dot.

Quantum dots differ from single-electron transistors in that the dots rely on specific quantum effects among a few electrons in logic circuits. Since the resistance of such devices is low, the precise number of electrons in the device is not known, and thus, cannot be used to store and retrieve information [193]. However, interactions between or among dots can. One quantum dot may affect another dot even if the two are not wired together. Two dots, separated by a large potential energy barrier, can influence each other through their long-range electrostatic interactions. For example, the electric field of the electrons in one quantum dot can change the number of electrons in another nearby quantum dot [179–181,238].

Adding an electron to one quantum dot will cause an electron to vacate a nearby dot, so long as the exiting electron can escape to a nearby location, as shown in Figure 9. The electron that started this chain of events must have tunneled into the first quantum dot from a nearby reservoir. Used in this way, a quantum dot can be thought of as a two-state device, with its two states corresponding to occupancy of the dot by zero or one electron. Two such devices placed next to each other would tend to take on opposite states, given that the electrons have a path of escape.

Lent, Tougaw and Porod [181,182] propose a clever variant of the arrangement of nearby quantum dots like those described above. By simply introducing more quantum dots to serve as the electron reservoirs, they suggest a five-dot "cell" that holds two electrons. The set of quantum dots is isolated from the surrounding environment by an insulating square constructed around the quantum dots. A schematic of two cells of this type is shown in Figure 10. Since the two electrons in each cell repel each other, they move naturally to opposite corners of the cell. As shown in Figure 10, the two such electron configurations possible represent the two states of the device.

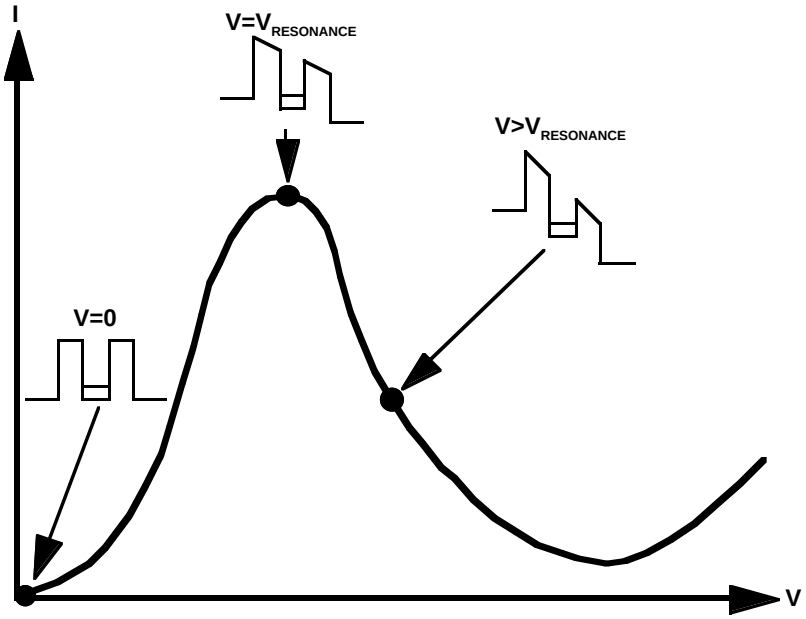

FIG. 4. Conductance Peak of an RTD. The current-voltage plot shows the peak conductance through an RTD is when the external potential V matches $V_{RESONANCE}$, an allowed energy state in the potential well. Figure adapted from Capasso [57].

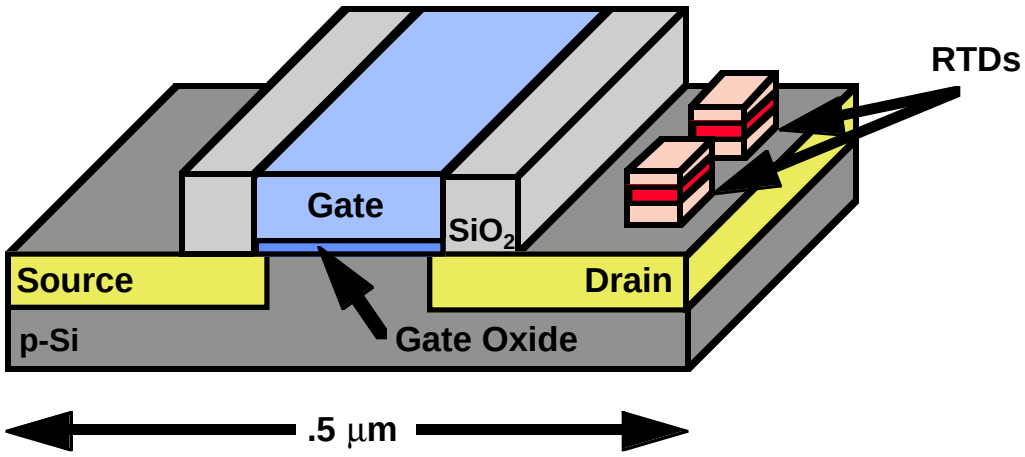

FIG. 5. Resonant-Tunneling Transistor. This is a hybrid approach to electronic nanocomputers that embeds nanometer-scale RTDs in the drain of a conventional microelectronic transistor to yield a multi-state device with a higher functional density. Figure adapted from work by Texas Instruments [246].

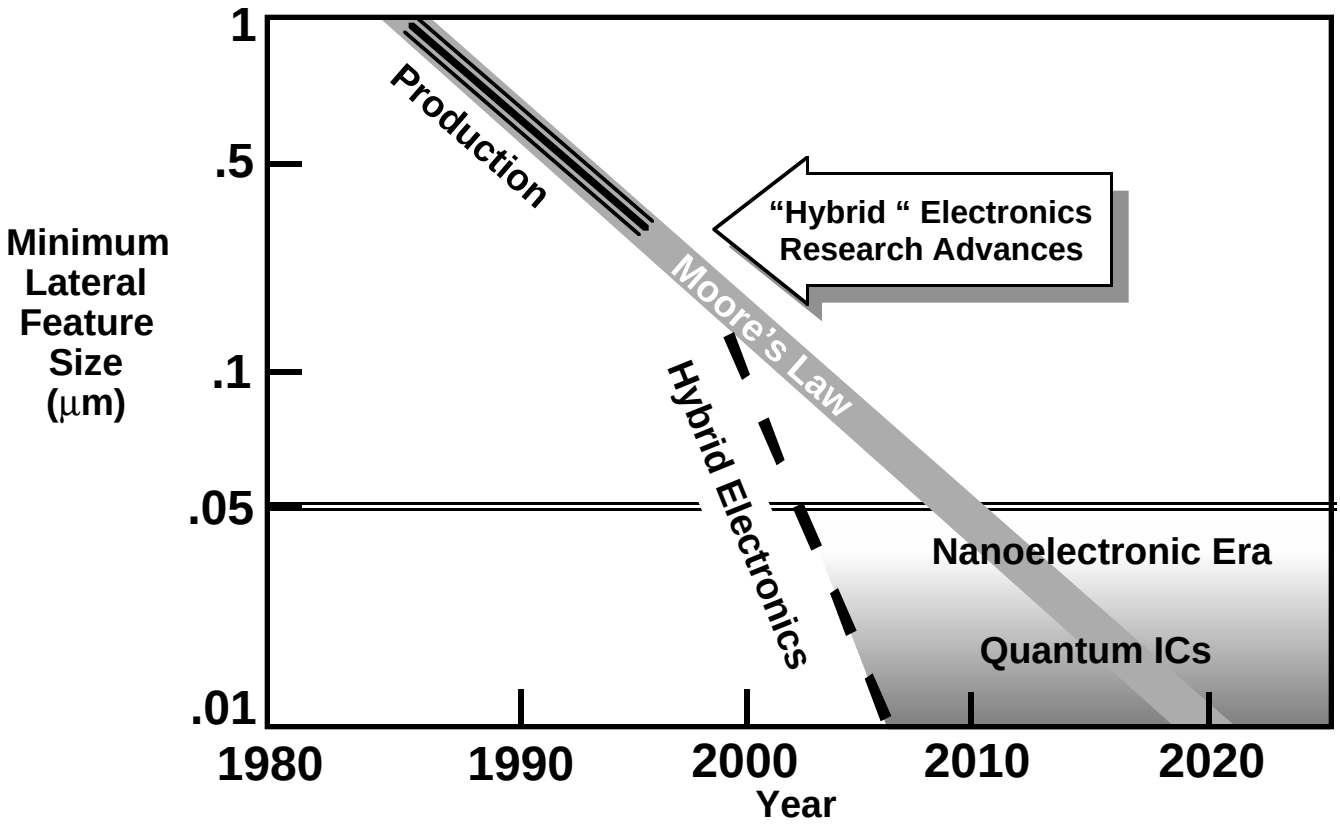

FIG. 6. Projected Timeline for the Arrival of Hybrid Nanoelectronics. Minimum feature sizes of devices may decrease at a faster rate than predicted by Moore's Law trend line through the use of "hybrid" nanoelectronic technology. Figure adapted from work by Texas Instruments [111].

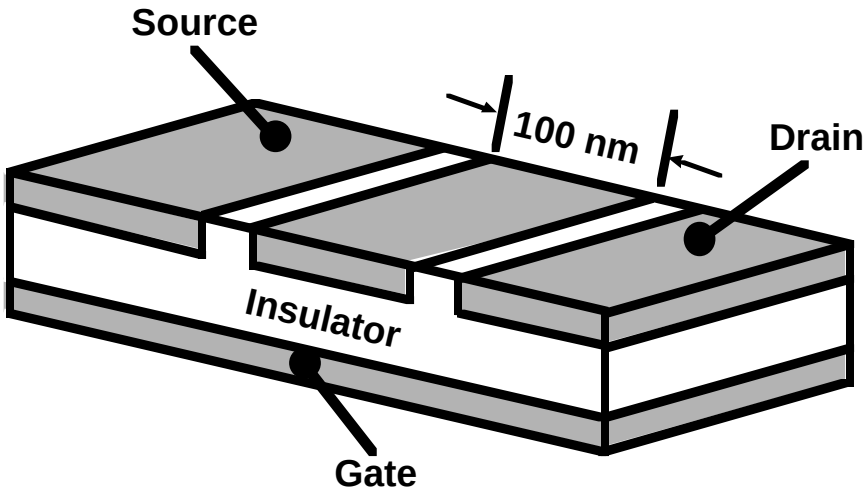

FIG. 7. Single Electron Transistor. Figure adapted from *Physics Today*, January 1993 [158].

Boolean logic functions can be implemented by setting up appropriate patterns of these Lent-Porod quantum dot cells. Since these quantum dot cells communicate via their electric fields (exchange of photons), and *not* through the flow of current (exchange of electrons), they are the basis for a new form of electronic computation. This and other approaches to "wireless" computation are described in greater depth in Section V of this paper, which discusses logic designs for electronic nanocomputers.

Difficulties associated with their fabrication present the primary obstacles to the implementation of computers based upon quantum dot cells. In order to compute without numerous errors, the location and size of the dots must be precisely controlled. The structures also must be carefully designed and prepared to minimize undesired tunneling of electrons across or out of cells. Also, as with single-electron transistors, the maximum operating temperature increases as the dots are made smaller, and any small background charge near a cell can permanently lock the cell into one position, ruining the computation.

D. Molecular Shuttle Switch

The devices discussed in the previous three sections all are nanometer-scale devices. In their presently realizable implementations, they are all composed of a very large number of atoms, however. It is possible, though, to make two-state devices, switches, that are composed of only one or a few molecules. For example, a research group at the University of Miami-Coral Gables reports the synthesis of a "shuttle switch" [46]. This switch consists of two interlocking molecules of the type that have been developed and refined in the pioneering work of the British chemist J. Fraser Stoddart [4,8]. As seen in Figure 11, the "shuttle" is a ring shaped molecule that encircles and slides (i.e., "shuttles") along a shaft-like chain molecule. Two large terminal groups at the end of the shaft prevent the shuttle ring from coming off of the shaft. The shaft contains two other functional groups, a biphenol group and a benzidine group, which serve as natural "stations" between which the shuttle moves.

The shuttle molecule contains four positively charged functional groups, which cause it to be attracted to sites on the shaft molecule with extra negative charge. For this reason, the shuttle spends 84 percent of its time at the benzidine station, which is a better electron donor than the biphenol station. The shuttle spends the remaining 16 percent of its time at the biphenol station.

The shuttle can be forced to switch to the biphenol station by the removal of an electron from the benzidine station. This process is known as electrochemical oxidation. Since both the altered benzidine station and the functional groups on the ring are positively charged, they repel each other. In this state, the shuttle spends most of its time at the biphenol station. By adding the missing electron back to the benzidine station, the switch will return to its original state.

There are a number of potential advantages to such molecular electronic devices. Large numbers of this type of device can be synthesized chemically at relatively low cost. Also, the small size of the device makes for extremely high packing density. However, the Miami group does not propose a means of probing the state of individual switches, though one route might be to use the shuttle to complete an electrical circuit. It is possible that this ring could complete a circuit in one of its two locations. In such an event, the rate of switching would be limited, at least, by the speed of electron transfer. Also, the mass of the shuttle molecule is very great compared to that of an electron. Thus the action of the switch would, necessarily, be slow compared to that of solid-state switches in which only electrons or electric fields (photons) move.

Although these switches would not be extremely fast, there could be a large number of them in a small area. In fact, these shuttle switches may pack into a three-dimensional lattice, creating an even larger space savings. Since this type of work is relatively new, there are many unresolved issues concerning the operation and application of such switches. However, the fabrication of a reliable molecular switch represents an important step forward towards molecular-scale computers.

E. Atom Relay

A team of Japanese researchers at the Hitachi Corporation reported the simulation of a two-state electronic switch of atomic dimensions [309]. The concept for this proposed device, termed an "atom relay," has some similarities to the molecular shuttle switch. In the atom relay, it is suggested that a labile atom rather than a shuttle molecule move back and forth between terminals or stations.

The atom relay would consist of carefully patterned lines of atoms on a substrate. The Hitachi simulations showed that a straight line of closely spaced atoms, or "atom wire," on the substrate is sufficient to conduct a small electric current. As shown in Figure 12, the atom relay consists of two atom wires connected by a mobile switching atom. If the switching atom lies between the two ends of the atom wires, the whole device can conduct electricity. However, if the switching atom is displaced from the two wires, a small gap is left in its place. In simulations, this gap is sufficient to reduce significantly the amount of current that can flow through the atom wire.

In order to move the switching atom in and out of the gap, the proposed atom relay has a third atom wire that passes near the switching atom. This terminal is called the "gate" of the atom relay because of its similarity to the gate of a field effect transistor. By placing a small negative charge on the gate wire, the switching molecule can be moved out of the atom wire. To move the switch-

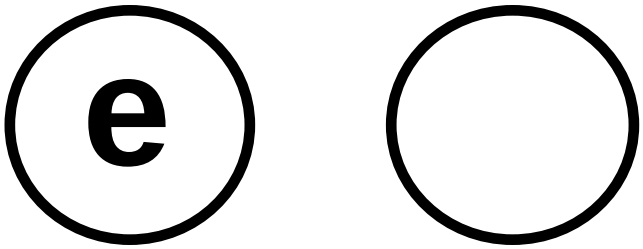

FIG. 8. Concept of a Quantum Dot. The rings represent "boxes" in which electrons are electrostatically isolated from the surrounding environment. Electrons can be added or removed from the quantum dots by adjusting the dot's electrostatic environment. The quantum dot on the left contains an electron "e", while the right one does not.

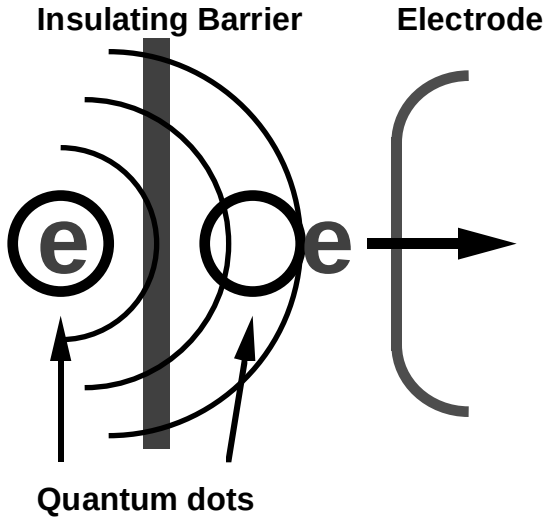

FIG. 9. Communicating between Quantum Dots. The electrostatic force of an electron in one quantum dot displaces an electron from another quantum dot on the other side of an insulating barrier. The displaced electron travels into the electrode.

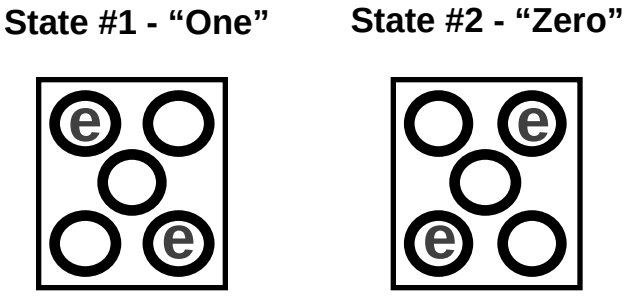

FIG. 10. Lent-Porod Quantum Dot Cells. Each quantum dot cell consists of at least four quantum dots, arranged at the corners of an insulating square that prevents electrons from leaving the cell. A fifth dot in the center improves the behavior of each cell, but does not affect its logical properties. The two electrons in each cell will exist in one of the two equivalent energy states depicted. These states can represent binary ones or zeroes [181].

ing atom back, a second gate called the "reset" gate, is necessary. The switch must be reset after every time it is used.

In an actual experiment that approximates this design, Eigler, Lutz, and Rudge report the creation of a bistable atom switch with the aid of a Scanning Tunneling Microscope (STM). In their experiment and in other related investigations, a xenon atom reversibly transfers back and forth between the tip of an STM and a substrate [92,258]. The location of the switching atom greatly affected the tunneling current that flowed from the STM tip to the surface. While the operation of the switch fabricated by Eigler's group is different from that of the theoretical atom relay, these experiments have shown that the movement of a single atom can be the basis of a nanometer-scale switch.

However, the designs for logic gates using atom relays would be limited to a two-dimensional plane. The Japanese group did not demonstrate how two separate atom wires could cross. Without crossing wires, only a subset of all possible logic functions can be implemented with these devices [207]. Individual relays have the advantage of being extremely small, on the order of 10 square nanometers. The speed of the relays would be limited only by the intrinsic vibrational frequency of atoms (10^{14} cycles per second), which is several orders of magnitude faster than present-day semiconductor transistors. Energy requirements, while not reported by the authors, would be rather low, resulting mostly from frictional forces between a single atom and the substrate.

On the other hand, not much energy would be required, either, to excite or evaporate a labile switching atom off the substrate and out of the plane of the atom wires, thereby destroying the switch. For this reason, it seems likely that very low temperature operation would be required if this device is employed.

It would be possible to fabricate atom relays with the aid of an STM. Since the relay's design requires a stable array of atoms for a long period of time, the question remains whether or not this is possible in the face of thermal drift. Both research groups predict that the switching speed is independent of temperature, so these stability problems also might be lessened if the devices are cooled to cryogenic temperatures. While switching based on atom movement has the advantages of high speed and low power dissipation, incorporating this mechanism into a more reliable device would improve its chances for practical applications.

F. Refined Molecular Relay

A more reliable two-state device based on atom movement might use the rotation of a molecular group to affect an electric current. The authors of this review suggest that the atom relay discussed in the last section might be refined and made more reliable by attaching the switching atom to a rotating group, or "rotamer." This rotamer would be part of a larger molecule that might be affixed to the same surface as the atom wires. See Figure 13 for a conceptual diagram of this arrangement (based upon a methyl-like group) and Takeda *et al.* [291] for a discussion of rotamers. By using the electric field of a nearby gate, the switching atom might be forced to rotate in or out of the atom wire. When the switching atom is in the atom wire, the conductance of the atom wire is high–i.e., the switch is "on." When the switching atom is rotated out of the wire, a second group will take its place. This replacement group will hinder the flow of current through the atom wire, causing the switch to be "off." A large third group on the rotamer could be used to prevent it from freely spinning due to thermal energy. Alternatively, hydrogen bonding might provide a resistance to spinning just adequate to "stop" the rotamer in the conducting position, but not so much that reversing the polarity would be insufficient to turn the rotamer.

Use of such a rotamer to effect atom switching is intended to stabilize and prevent the evaporation of the mobile switching atom. This might alleviate one of the principal weaknesses of the atom relay discussed in the previous section. The refined molecular relay has some similarity in its mode of operation to the shuttle switch described in Section IV D. The rotamer in the refined relay is likely be more sensitive to energetic perturbations than the molecular shuttle, though, because the rotamer is likely to be lighter and have a much smaller range of motion between switching positions. The molecular relays and the shuttle switch are a kind of hybrid between electronic switches and the molecular-scale mechanical devices described by Drexler [88], Merkle [218], and others.

One of the disadvantages of a rotating switch based upon a methyl-like rotamer group is that there are three different switch positions associated with the three groups attached to the rotamer. A more suitable molecule might be one that moves back and forth between only two distinct states. An example of this type of molecule would be cyclohexane, or one of its substituted derivatives. Cyclohexane can bend into two different forms, commonly known the "boat" and "chair" conformations [168,264]. As shown in Figure 14, a voltage on a nearby gate might force the cyclohexane switch into one of its two configurations, affecting the conductivity of a nearby atom wire. The cyclohexane-type molecule could link to a molecular framework while the remaining ring carbons have substituents tailored to use steric repulsions or chemical attractions to reduce false switching caused by thermal energy, while also sterically protecting the conducting atom from chemical attack.

These two designs should operate at speeds governed by molecular rotation, which typically occurs at frequencies in the vicinity of billions of cycles per second–i.e., the GigaHertz (GHz) regime. This is slower than the atom switch, but the design may be much more reliable. The

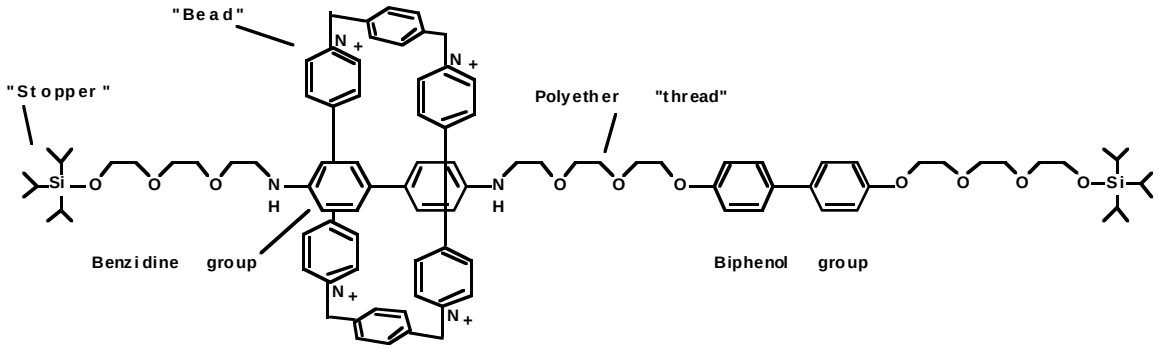

FIG. 11. Reversible Molecular Switch, Bissel *et al.* [46]

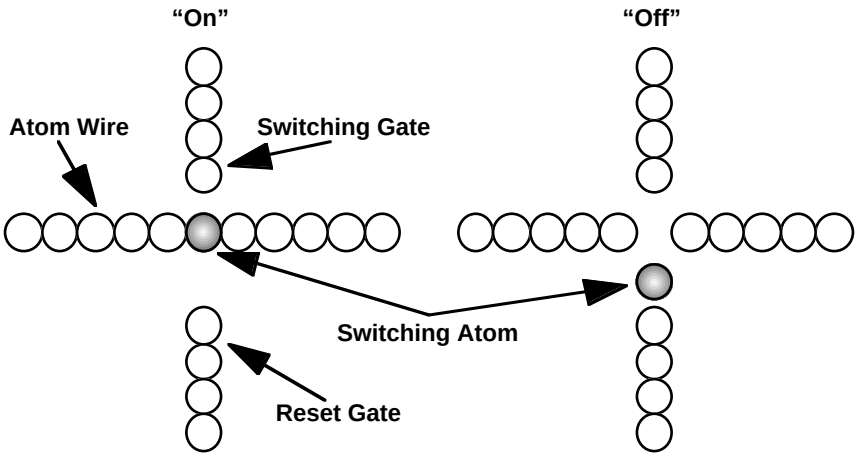

FIG. 12. Atom Relay, Wada *et al.* [309]

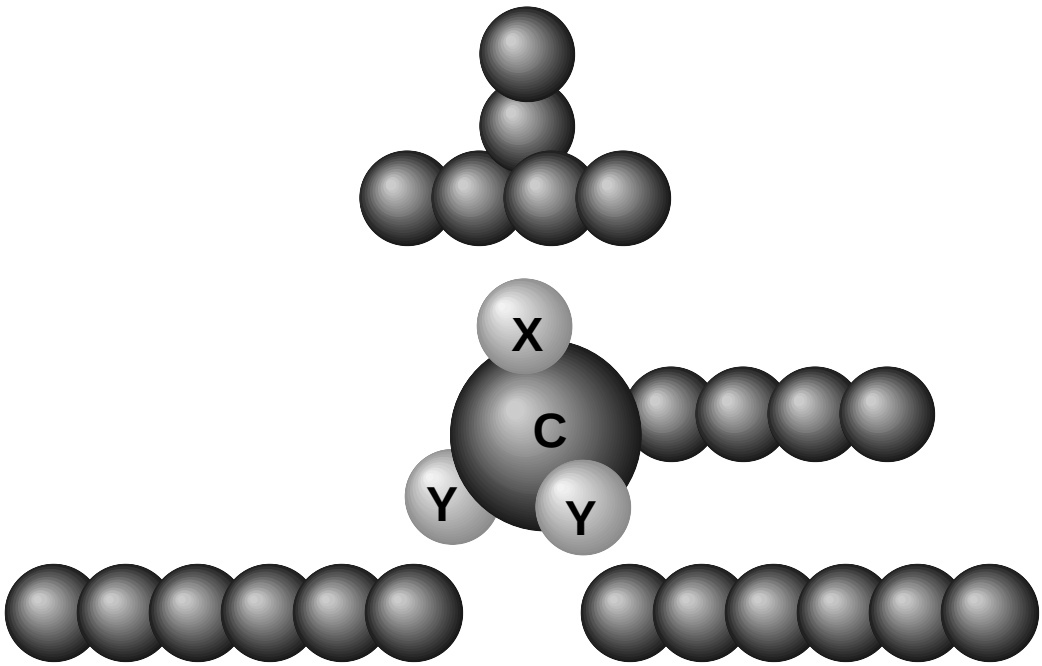

FIG. 13. Refined Molecular Switch, Type 1

packing density of these refined relays is likely to be much greater than that for a two-dimensional design, and the energy dissipated in their operation ought to be very low, primarily arising from breaking weak van der Waals attractions and/or hydrogen bonds.

V. LOGIC DESIGNS AND ARCHITECTURES FOR ELECTRONIC NANOCOMPUTERS

The most open-ended problem presently challenging the realization of nanoelectronics is the development of the logic designs and computer architectures necessary to link such small, sensitive nanodevices together to perform useful calculations efficiently. This must be done within a structure that can be increased in density to contain between 10^9 and 10^{12} functional logic units in an area or volume smaller than that achievable in today's integrated circuits. Because of this density and the small scale, it is unlikely that we will continue to use the designs–i.e., the connective topology–of present-day microelectronic logic [109]. However, the issues that must be addressed for connecting together very many nanodevices for the purpose of computation are not as clearly defined yet as the relatively clear-cut (though difficult) issues facing designers trying to improve individual nanodevices.

An effective nanocomputer architecture must fall within the bounds of certain fundamental limits, though. Once a global architecture is decided upon, specific problems such as electromigration, high interconnect resistance, significant crosstalk, and error correction requirements may impede its implementation. Nevertheless, room exists for exploring powerful new architectures with which to build nanocomputers. Examples are the "wireless" logic designs that have been proposed recently. These may provide a solution to at least some of the problems that would plague nanometer-scale variants of more traditional architectures. In this section, a few of the new proposals for wireless nanometer-scale logic are discussed as well as some of the key constraints upon nanocomputer logic designs. In Table II, these wireless logic designs are compared with more traditional electronic-computer logic designs using wires.

A. Wireless Ground State Computing

Recently, Craig Lent, Wolfgang Porod, and their collaborators at the University of Notre Dame proposed a method for computing that does not involve traditional wires to propagate information. Their design depends on the dynamics of direct, local interactions between devices and their neighbors. This type of design is called a cellular automaton [131,296,320]. The Lent-Porod quantum cellular automata (QCA) scheme would be composed of many quantum dot cells seeking the lowest energy state, or "ground state," for the entire assembly of cells [180–183].

As outlined above in Section IV C of this paper and depicted schematically in Figure 10, Lent and Porod have suggested constructing a two-state cell made of quantum dots. The two electrons can exist inside the cell in two equally probable, low energy configurations or states. These two states can represent a binary zero or one. The state of an individual cell can be fixed by applying an appropriate voltage on an external probe or gate.

The polarization of a cell to a particular state is a signal analogous to a high or low voltage on a wire within a conventional integrated circuit. This signal can be propagated by creating a row of quantum dot cells. If a cell with a fixed state is next to a cell with a different configuration, the cell with the different state will change its state to match the cell with the fixed state. This corresponds with a reduction of the energy of the system as illustrated in Figure 15. The transmission of a signal between a pair of cells may be extended through a row of many cells to create a "wire" of cells. Note that in the transmission of the signal from one cell to another, there is no exchange of electrons between adjacent cells. Signals are passed between neighboring cells through the influence of the electric fields of the electrons contained in the quantum dots. The electric field of the electrons in the quantum dot travels at the speed of light, and so the time required for one electron to influence another is negligible. A slower relaxation time is required for a change in the electron configuration of each cell in the chain. However, this process may be as fast or faster than the passage of current or voltage along a sub-micron metal wire in a conventional computer design. Sub-micron metal wires have high resistance and, therefore, take a long time to change between high and low voltages.

Rows of quantum dot cells can perform two tasks common in conventional integrated circuits. First, rows of cells can carry signals over long distances just as aluminum or doped silicon wires do in circuits. Second, rows of quantum dot cells also should be able to amplify weak signals to discrete states, a very useful feature of conventional digital circuitry. Quantum mechanics allows each electron to be spread over more than one dot within each cell. Thus, the charge in a single cell might not be fully localized along one diagonal. Signals would not always be a discrete zero or one. However, as each row is lengthened by the addition of more cells, the polarization of the cells should rapidly approach–i.e., be amplified to–more "perfect" zeros or ones.

In addition to a straight wire-like line of cells, one can use quantum dot cells to build corners, fan-out junctions, and inverters, all of which are building blocks of digital circuits [181]. "Wires" carrying signals can cross each other in the plane without interference. However, logic gates more complicated than inverters are not so simply translated into this new design.

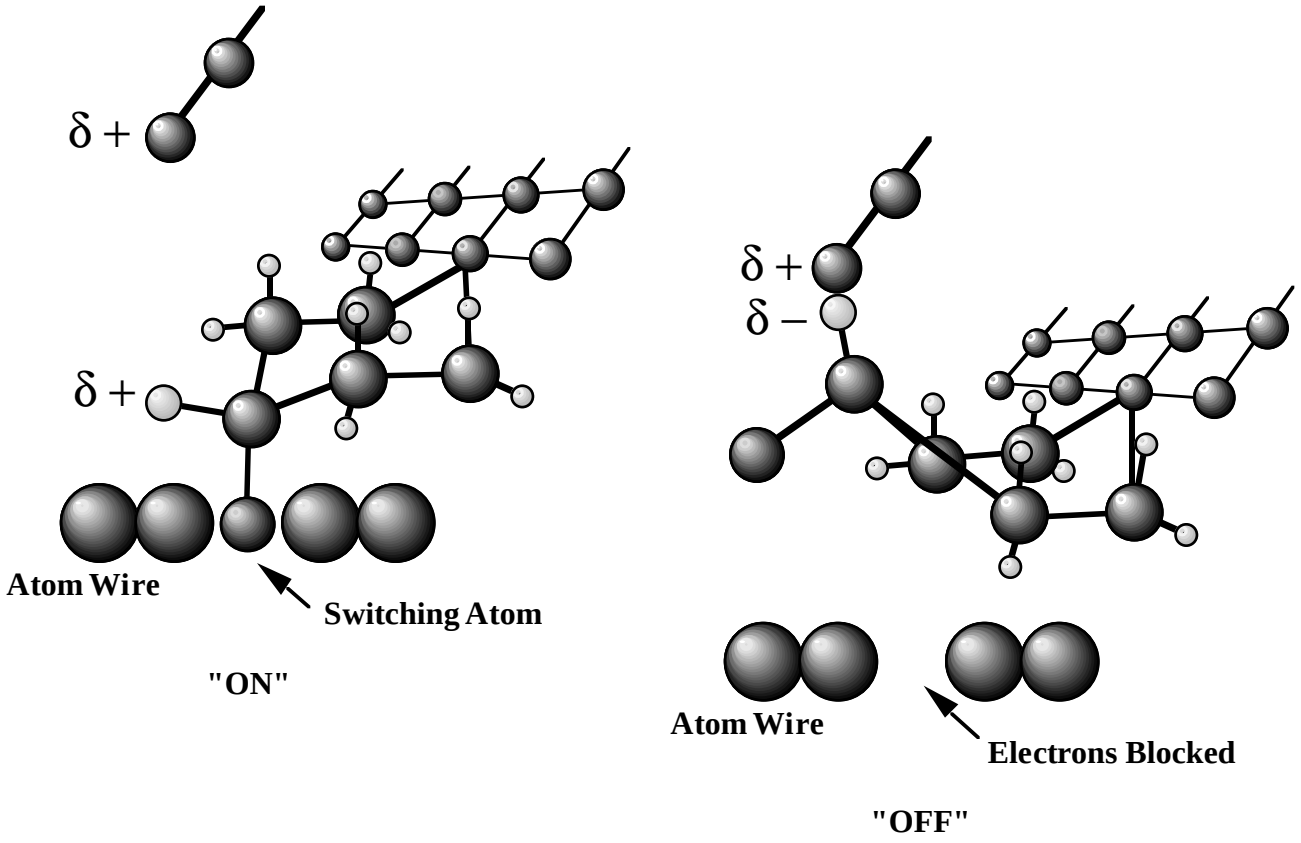

FIG. 14. Refined Molecular Switch, Type 2

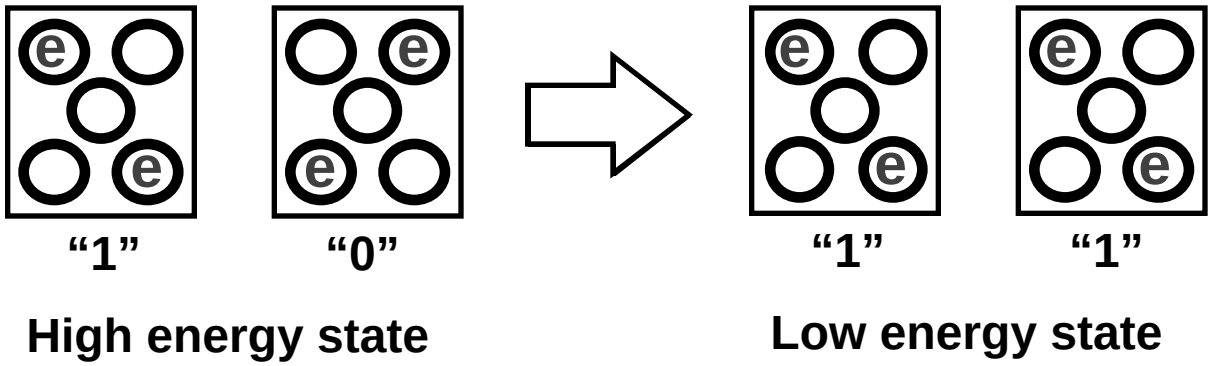

FIG. 15. Communicating between Quantum Dot Cells. Quantum dot cells do not communicate by the transfer of electrons, but by the electric fields of their electrons. In general, a high energy state exists when two electrons are in close proximity to each other due to the repulsive forces of their electric fields. When the electrons are moved away from each other, the system moves to a lower energy state. Therefore, when two quantum dot cells are in opposite states, the energy of system is reduced by shifting so that both cells have the same state. Thus, information is transferred from one cell to the next.

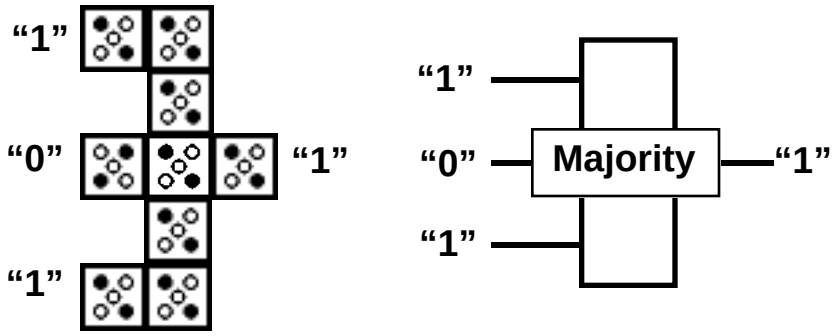

FIG. 16. A Majority Gate Constructed with Quantum Dot Cells. A simple majority gate can be implemented using quantum dot cells. The gate determines the output based on the input value that is in the majority [182].

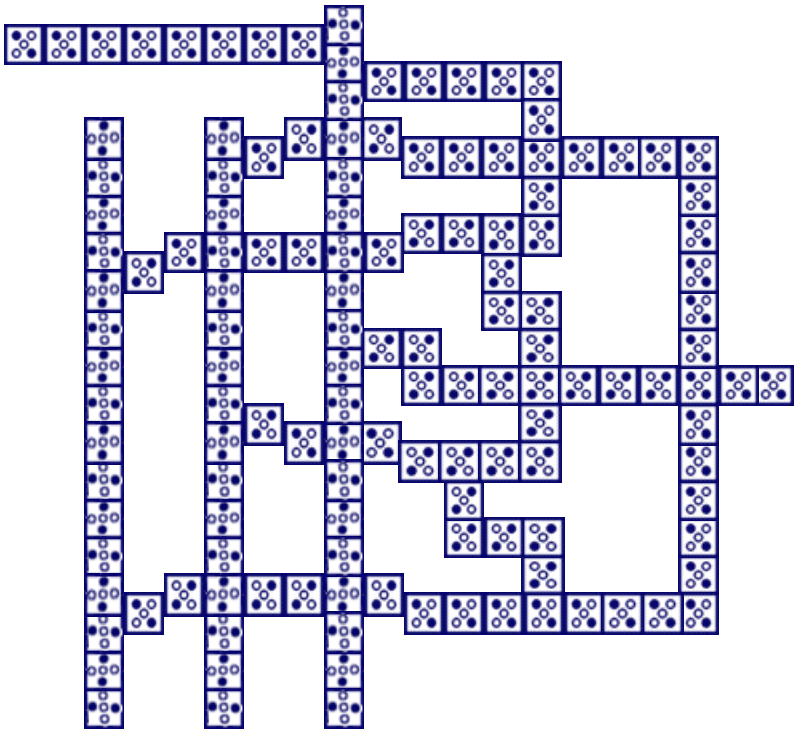

FIG. 17. A Full Adder Constructed with Quantum Dot Cells. A full adder is a common circuit in digital logic on microprocessors. It adds together three one bit numbers. Such a circuit can be implemented using the quantum dot cells and the majority logic illustrated in Figure 16 [182].

The basic logic gate in the quantum dot cell logic design is a *three*-input "majority" gate, shown in Figure 16. The output of this gate is zero or one, corresponding with the value of the majority of the inputs. For example, if two or three of the inputs are zero, the output also will be zero. Such majority logic gates can implement any logic function. By fixing one input of the majority gate to a 1, the output corresponds to the OR of the two remaining inputs. Alternatively, by fixing one input to a 0, an AND gate can be made.

Still more complex logic structures can be constructed with the quantum dot cells. As depicted in Figure 17, it is possible to make a "full adder" logic structure. This full adder contains 138 quantum dot cells, corresponding to 690 quantum dots, given 5 dots per cell. If the center-to-center distance between dots within a cell were 20 nanometers and the dot diameter 10 nanometers, a single full adder could fit in an area of approximately 1 square micron. The feature sizes required to make such small quantum dot cells would require very aggressive application of today's technology. It is possible with today's electron-beam lithography, though [119]. By contrast, the semiconductor industry projects that in 2010 the maximum packing density for transistors will be only about one per square micron [275]. Conventionally, it requires approximately forty transistors to build the same full adder.

The dramatic advantage in projected density for quantum dot cells is explained by two factors. First, much of the space in a conventional integrated circuit is taken up by wiring, which is unnecessary in the quantum dot cellular architecture. Second, the width of a single cell is only a few times the minimum feature size of the fabrication process, as compared to the proposed 1 micron diameter of a transistor complete with wiring, which is 14 times the proposed minimum feature size [183]. It also may be possible to make the *entire* quantum dot cell chemically [60]. This could increase the packing density even more.

The output of Lent-Porod quantum dot logic arrays is determined by the minimum energy state, or ground state of the entire system of quantum dots. In other words, as the calculation progresses, all the quantum dot cells will align themselves, such that the energy of the whole system is as low as possible. The time required for the quantum dot cells to compute is limited only by the length of time needed for the array of cells to "relax" to its minimum energy or "ground" state. For this reason, this type of computation often is referred to as "ground state computing."

It follows from the preceding that one of the disadvantages of these quantum dot computers is that signals could not only travel forwards, from input to output, but could also travel backwards. Each cell exerts its electric field on the cells both before and after it. This feature often makes the design of large logic structures very difficult. Lent and Porod have offered some simple design rules so useful logic devices can be designed with quantum dot cells. Ideally, individual majority logic gates could be combined to make larger logic structures. The outputs of such larger structures would be determined according to the simple rules for determining the output of the component majority gates.

However, such simple design rules can produce logic that does not work as expected or predicted by the rules. This problem is illustrated in Figure 18. Figure 18(a) shows a logic structure that can be made using quantum dot cells. The logic structure consists of three consecutive majority logic gates fed by three fixed inputs. According to the definition of majority logic gates, the output of the logic structure should be a "1." Figure 18(b) shows the circuit (with the initial inputs) as implemented using the Lent-Porod design rules. As discussed above, the entire structure will adjust to minimize the energy of the system. That is, each cell will minimize the repulsive interactions with its neighboring cells by matching its polarization to that of as many of the adjacent cells as possible. As a result, the number of "mismatches," or adjacent cells with opposite polarizations, will be minimized *throughout* the logic structure. According to the local design rules for the individual majority gates, the logic structure should settle with an output of "1," as shown in Figure 18(c). This produces the three mismatches shown in the shaded regions of Figure 18(c), one at each majority logic gate. However, this is not the lowest energy state possible for the system. As shown in Figure 18(d), a valid state with only two mismatches (in the shaded regions) can be reached by this aggregate logic configuration. This yields an output of "0," a different one than predicted by the locally applied design rules.

The true global ground state for a quantum dot cell logic structure such as the one in Figure 18 would be the one with the minimum number of mismatches. The dynamics of the switching within the entire logic structure may push the system to the higher, three-mismatch energy state associated with the configuration shown in Figure 18(c). However, it is not clear that the system would remain in that state for a sufficient amount of time to read the "correct" output. Given time, the system would prefer to settle in the lower, two-mismatch energy state shown in Figure 18(d). Unlike traditional microelectronic logic circuits, each logic gate in a ground state computer would be dependent on both future computations (i.e., those closer to the outputs) and past computations (those closer to the inputs). This makes the design of any circuit for a ground state computer a somewhat more difficult task.

High ambient temperatures also might plague quantum dot cell architectures. As the energy value kT (where k is Boltzmann's constant and T is the absolute temperature) becomes comparable to the energy difference between two states that differ only by the "correct" or "incorrect" polarization of a single quantum dot cell, there is a significant probability that the system will be found "excited" in the incorrect, higher energy polarization state. For a 20 nanometer dot-to-dot distance, this energy associated with an error in one cell's polarization

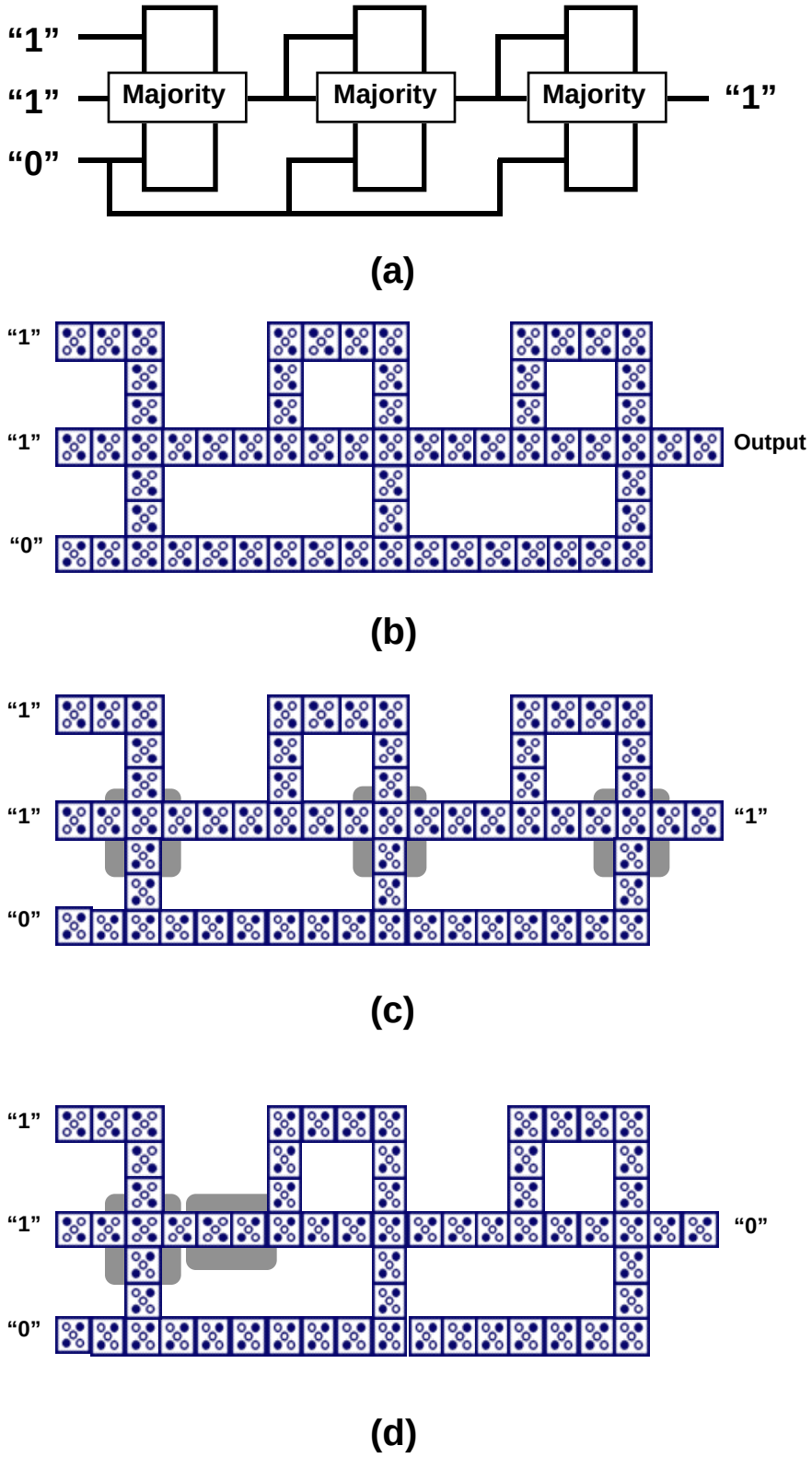

FIG. 18. Example of a Difficulty Encountered in the Design of Ground State Computers. A simple circuit using three majority gates can be constructed and implemented using Lent-Porod design rules as seen in parts (a) and (b). With the given inputs, the output expected is a "1." As shown in (c), the circuit giving the expected answer would contain three mismatched cells, highlighted with grey boxes. However, the true ground state contains only two mismatches, and would give the incorrect answer as shown in (d).

would be 1 millielectron volt, or one twentieth of thermal energies at room temperature. Thus, thermal fluctuations are likely to be a major problem. Even if the error energy could be made many times larger by making the individual dots smaller and closer together, entropic effects could limit the size of an array of cells. Arrays of cells might have to be operated at very low, cryogenic temperatures to reduce the impact of thermally induced fluctuations.

There have been other reservations expressed regarding wireless cellular automata designs [5,22,193]. Among these reservations is the possibility that such designs may function only for very, very precisely tuned values of the controlling external parameters. This might make cellular automata hard to fabricate in practice and very sensitive to external perturbations. Also, it is asserted by some scientists that even under the best of circumstances, these computers would be very slow because of the significant time required for the system to collapse to its ground state [5]. However, these objections to wireless ground state computing are founded, to a great extent, in arguments based on static interactions among cells. They may not take sufficient account of the dynamics of a row of quantum dot cells [186]. Despite some potential technical problems with the Lent-Porod scheme, it does suggest an approach for bypassing some of the seemingly insurmountable scaling problems associated with the wiring in conventional electronic computers. Improvements upon this logic design, such as the ones that are discussed in the next section, could help push electronic computing technology towards a fast, energy efficient, and realizable design for an electronic nanocomputer.

B. Modifications of Wireless Computing Designs

A number of modifications have been proposed to remedy some of the known problems with the basic wireless computing design described above–especially the predictions that such designs may be slow and also prone to becoming "trapped" in energy states other than the ground state. One such proposal is due to Lent and Porod themselves [184]. Another is due to Korotkov [170]. The details of these two proposed modifications are very different.

1. Lent-Porod Adiabatic Wireless Computing Approach

A serious concern for wireless computing with quantum dot cells is that that a system might become "trapped" in metastable states corresponding to local minima in energy [5]. In that case, the computer might never relax to the true energy minimum corresponding to an expected computational result. More often, it might relax to the minimum energy, or correct result, but at an unpredictable rate. Lent, Tougaw, and Porod have pointed out that this concern might be addressed, though, by introducing adiabatic switching into the quantum dot cellular automaton [182]. Lent and Porod have provided details for a scheme in which the system is allowed to move adiabatically to a lower energy state from the high energy state produced when the input voltages are applied. Energy dissipation would play no role in this process. Via such adiabatic switching, the unpredictable speed of dissipative relaxation mechanisms might be avoided to give better control of the computing process using quantum dot cellular automata [184].

2. Korotkov's Wireless Dissipative Computing Approach

Korotkov [170] suggests a wireless design that does not use Lent and Porod's quantum dot cells. Instead, it uses arrays of individual quantum dots organized into sets of wire-like local elements. A key feature is its expenditure of small amounts of energy in a dissipative process to drive the wireless computer rapidly toward a lower energy state that represents the result. A certain amount of heat may be dissipated safely even when a number of devices are packed together in a nanometer-scale area or volume. In so doing, Korotkov, Likharev, and their collaborators attempt to retain the strengths of nanometer-scale wireless quantum logic based upon cellular automata, while resolving some of the difficulties associated with the Lent-Porod ground-state computing design.

As discussed above, one of the problems with ground state computers is that every calculation is dependent on the *entire* system of quantum dots and electrons. Alternatively, by subdividing the wireless computing structure into different, loosely coupled parts or elements, the different elements of the structure can be forced to relax *locally* to a lower energy state. Then, one initial local change in state can induce another neighboring element to change its state, and so on, in sequence, across a chain of such elements.

The wireless structure that Korotkov and his collaborators have suggested to generate this sequential process is depicted in Figures 19 and 20. Each local element mentioned above is a row of quantum dots. A neighboring element is a second similar row of quantum dots perpendicular to the first. The entire chain of elements is placed in a global electric field. A signal is propagated by the formation of electron-hole pairs in each row of quantum dots. The electric field allows the local polarization of the electron-hole pair in one element which in turn induces the formation and polarization of a pair in the next element. (See reference [105], Lecture 14, page 3 for a clear discussion and explanation of electron-hole pairs.) Therefore, chains of elements could be linked together to create wire-like structures through which external inputs at one end quickly propagate to the other end without any flow of current.

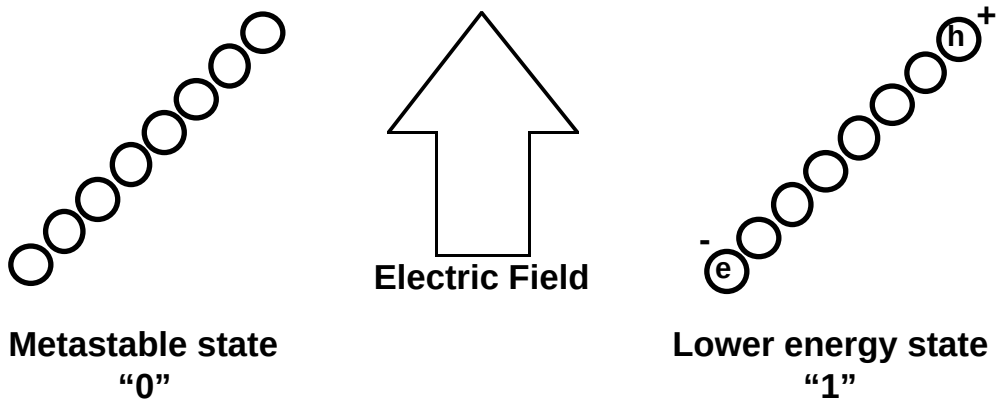

FIG. 19. Elements of Korotkov's Wireless Dissipative Computer. The elements of Korotkov's dissipative computing scheme are rows of quantum dots in an electric field. The two possible states of a row of dots is shown here.

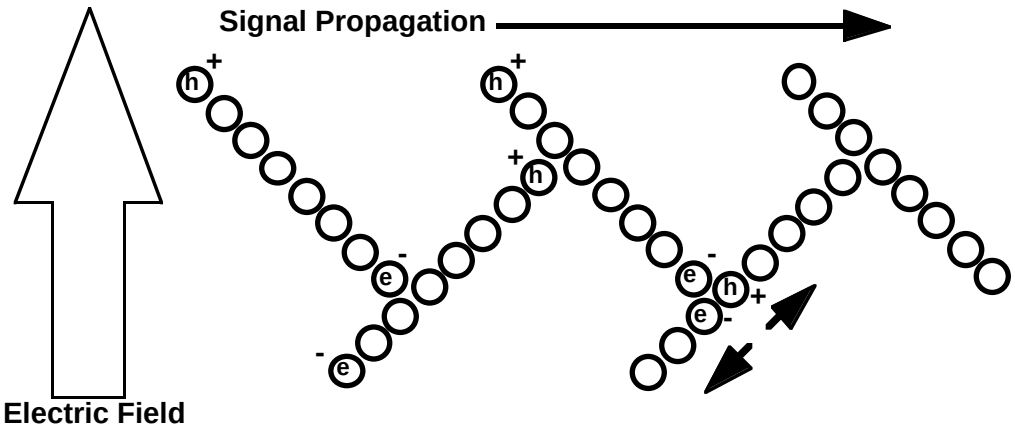

FIG. 20. Operation of Korotkov's Wireless Computer. Sequential polarization of a succession of the elements depicted in Figure 19 can transmit signals across a substrate without a flow of electrical current [170].

However, Korotkov's wireless dissipative computing scheme must overcome certain challenges that may make it difficult to implement. Just as with single-electron transistors discussed above, the switching transition of the quantum dot chains is triggered by a single nearby charge. Unlike ground state computers which, in principle, could recover from transient noise by returning to the ground state, dissipative computers do not have any such built-in error correction. This could make such computers vulnerable to premature triggering by transient electrical noise such as a charge moving around in the substrate or insulating layer of a solid-state quantum dot.

Another problem with this logic design is that the magnitude of the applied electric field must be chosen so that the metastable "zero" state, where all quantum dots in a single element are uncharged, is sufficiently stable to persist indefinitely in isolation. However, the metastable state also must be sufficiently close to instability so that a single nearby charge triggers the element to fall to the lower energy state. There is a narrow range of electric field strengths, approximately 5 percent of the total field strength, that would satisfy both of these criteria. This constraint on the ranges of the useful field constraints would be even narrower if lack of precision in the fabrication process prevented all of the quantum dots from being exactly the same shape and size. Experience with 0.5 micron dots in a gated semiconductor heterostructure shows that 50 percent nonuniformity in the number of electrons held in an identically-processed dot is common. This problem might be mitigated, however, with more uniform molecular electronic structures.

C. Adaptations of Wireless Computing Designs

There also have been adaptations of the Lent-Porod wireless quantum dot cell computing scheme to permit the design of proposed nanocomputers based on neural network design rules [132], rather than those for cellular automata. Lent and Porod themselves have proposed such a neural network design [185,300]. The research group at Purdue University also proposes a nanometer-scale neural network design using molecular wires to connect devices [22]. Nanometer-scale neural networks may open up a new domain for non-digital logic designs.

1. Quantum Cellular Neural Networks

The Lent-Porod proposal for quantum cellular neural networks (Q-CNN) would construct a nanometer-scale *analog* neural computer from quantum dot cells, rather than a digital quantum cellular automaton (QCA). A Q-CNN would use to its advantage the same device rules for local communication between cells as stated for the QCA. In addition to its two-state polarization, each cell would have a quantum degree of freedom (a phase difference) associated with it. However, the synaptic inputs, or interactions between cells, still would depend only on the cell polarizations as in the quantum cellular automata design. The phase information would be localized within each cell. It would be required to retain information from one time to the next. Cellular neural networks offer an advantage over fully interconnected neural networks because they use primarily nearest-neighbor interactions, as opposed to global interactions over relatively longer distances.

2. Nanometer-Scale Nonlinear Networks

Nanometer-scale nonlinear networks (NNN) such as the Q-CNN design summarized above are among the proposals for circumventing some of the drawbacks of computing with cellular automata [22,25,32,256]. One proposal of an NNN is due to Balasingham and Roychowdhury [22]. It would use arrays of interconnected nanometer-scale metallic islands to perform computational functions via nonlinear interactions among thousands of elements of the array. Some of the advantages that may accrue to this approach are as follows:

- NNNs do not require lithographic wires.
- NNNs take advantage of nonlinearities inherent in charge transport via molecular scale or nanometer-scale links, and make them contribute to the computation.
- Preliminary modeling seems to indicate that these NNNs can perform both computational and memory functions [22].

D. Considerations and Constraints for Nanocomputer Logic Designs

The preceding proposals for new nanocomputer designs should be considered with certain architectural issues in mind. Designs for electronic nanocomputers must be able to address several major questions and constraints. These constraints are enumerated and discussed below.

1. Approaches to Parallelism

How will a nanometer-scale computer approach a computation? This is the first question to be considered in designing a nanometer-scale architecture. Will the computer divide a given problem into smaller portions to be worked on by many separate devices connected in parallel, as in today's high performance computers, or will the machine search the entire solution space, trying each

possible solution for the whole problem separately in parallel? The approach to the solution will determine major features of the type of architecture developed [109].

2. Interconnects

In communicating between nanoelectronic devices, what types of interconnects will be used? The lifetime of the computer and/or the speed of computation will be dependent on the type of connections used between devices. Some types of nanodevices, such as single-electron transistors, resonant-tunneling transistors, and some molecular devices, could be connected to circuits with metal wires in a fashion similar to today's MOSFETs. The designs for logic circuits using such devices may not have to be modified extensively [171,305].

However, there are disadvantages to continuing to connect much smaller, two-state (or multi-state) devices with metal wires. For example, in Intel's Pentium *micro*processor, seven layers of aluminum form a knotted canopy of wires above the plane of the transistors themselves. Conventional metal wires implemented on the scale of the nanodevices will not work due to the electromigration of atoms. Electromigration is caused by a stream of electrons flowing through the metal wire and pushing atoms at the junctions of the metal crystal grains "upstream." Conversely, atom-sized holes in the system move "downstream" to the end of the wire where they accumulate until the wire is broken [207].

Even if features on conventional devices (or their nanometer-scale variants) shrink to 70 nanometers by 2010, as projected by the semiconductor industry [275], wiring constraints could limit the packing density to one transistor per square micron, only a few times more dense than that achieved today [183]. Concerns about reliability already limit the minimum diameter of metal wires. Submicron wires may fail after only 100 hours of operation, torn apart by the electrons coursing through them [175]. Electromigration might be avoided if the metal wires were composed of a single-grain metal crystal [207] or if *molecular* wires were used with lower currents.

Despite the possibility of developing more reliable submicron wires, their higher resistance and long length could drastically limit computing speed [207,274]. Also, if the wires are closely packed, their mutual capacitance is likely to cause severe crosstalk. Signals on one wire will induce signals on other nearby wires. Moreover, the danger of electrons tunneling from one wire to the next limits the density of wiring. In the past, scaling down the dimensions of computers has increased the speed at which they operate. However, because of the limits imposed by long, thin wires, computing soon may reach the point where smaller computers are no longer faster computers. Even logic using electronic nanodevices may not be faster than that using equivalent microelectronic devices. This is because one approaches a lower limit on the time required to charge and discharge wires, interconnects, and other structures as they become small compared to the wavelength of a moving electron [193].

An alternative to wire interconnects is through direct interdevice communication. The wireless logic designs discussed above are examples of how logic could be constructed to operate using many fewer connections. Using such "wireless" logic, wires still may be needed to communicate between the edges of logic gates and over other relatively long distances across a processing unit. However, no wires (or very few wires) would be needed for connecting points inside the wireless logic gate. This would drastically reduce the number of wires that need to be accommodated in an ultra-dense computer.

This advantage accrues from the fact that wireless logic gates, like those described above, are "edge driven." An edge driven processor is one that inputs and outputs information only on its edges. All of the computation proceeds in the middle of the processor using the information passed from the edges by local currentless interactions (e.g., electric fields). This is an efficient means of communicating with the processor since relatively few devices in the interior of the logic structures are addressed directly.

However, wireless computing may slow down the speed of the propagation of information, and, therefore, slow down the processing speed of a nanocomputer. Unlike conventional wires that carry information at a rate independent of the computer's processing cycles, the information in a wireless system must pass through the nanodevices themselves. Their information transfer rates may be bound intrinsically to the clock cycles of the computer. In a processor with m devices, the number of cycles required to propagate the information would be $\sqrt{m}$ [207]. Thus, for large numbers of devices with no wires to transport information, a large number of clock cycles would be necessary to propagate a signal across the system. Hence, a slowdown in processing speed would be expected.

3. Error Correction

How will intrinsic errors in computed bits be corrected? This is perhaps the most important question for the design of architectures for nanocomputers. All computers must correct errors created by their devices. In general, component devices have a fixed rate of error generation that determines the probability of failure of the entire computer. In order to decrease the probability of failure, individual devices must be made more reliable or circuit redundancy must be built into the design. In conventional computer architectures, the greater the redundancy, the less chance the computer will give incorrect outputs. It is necessary to include redundancy in nanocomputer designs, as well, since the intrinsic probability of error in nanodevices is likely to be high. This is due in part to the probabilistic nature of quantum mechanics that govern their operation [12,19,102,105,207].

How much redundancy is necessary before the nanocomputer is considered "reliable"? It is likely that increasing redundancy would reduce both the errors and the computational speed [43,207]. The increased computational speed expected from nanocomputers may need to be balanced against the necessity for ensuring the reliability of the computations. The question becomes, what is the proper balance? Redundancy also reduces some of the functional density that otherwise may accrue from increased device density. It seems possible to have nanometer-scale computers much more dense functionally than today's microcomputers. However, the order of magnitude of the increase in density will be dependent on the degree of redundancy needed to ensure error correction and fault tolerance.

The best logic designs for electronic nanocomputers will be those that construct logic using advantageously the quantum mechanical domain in which the component devices of such computers would exist. Nanodevices are generally simple nodes that retain state information. Connecting such nodes in modular, web-like designs seems desirable [131]. Such designs–e.g., QCAs and NNNs–would use short interconnects, communicating information only over short distances. Input and output could be edge driven in systems with local interconnects [6]. This avoids addressing each device individually. Thus, a number of proposed nanocomputer logic designs rely on cellular automata-like interactions or neural networks [6,22,109,131,180–183,185,295,297].

VI. FABRICATION

Ultimately, the "best" technology or design from which one can construct a nanocomputer may not be the one that ensures optimal computational performance. Rather, the nanometer-scale technologies and designs of choice will be those that function effectively and also can be fabricated most economically, reliably, and safely. Improved fabrication technologies plainly are the key to progress in nanotechnology and nanoelectronics. To some extent, fabrication technologies control even the ideas investigators permit themselves to think and propose. Certainly, no matter how small a proposed electronic device can or should be built in theory, the limitations in fabrication processes determine how small the device can be built in practice.

In consequence, great effort and resources have been applied in recent years to advance techniques for the fabrication of nanometer-scale structures. There has been a correspondingly great increase in the sophistication and flexibility of the techniques with which truly nanometer-scale structures can be fabricated [155,303,317]. This great improvement in fabrication capabilities at the level of the most fundamental structural elements of matter is of great significance, perhaps of greater significance than the development of the nanometer-scale computers for which these techniques nominally are being developed.

Present techniques for the fabrication of nanometer-scale structures can be broken down into four main categories:

- Lithography
- Molecular Beam Epitaxy (MBE)
- Mechanosynthesis with Nanoprobes
- Chemosynthesis

Lithography and MBE are more traditional methods employed by the semiconductor industry to fabricate microstructures in present-day, very-large-scale integrated (VLSI) circuits [55]. With refinements, these processes could be honed to fabricate nanostructures as well [145,208]. Lithography uses a beam of light or matter to make a pattern on a surface, which then is refined or "developed" into a structure using bulk chemical processes. MBE uses a precision beam of atoms or molecules to deposit structures on a surface layer-by layer, where the layers are built up slowly as the beam moves relative to the surface in a carefully controlled pattern.

The newer, emerging fabrication technologies of mechanosynthesis with nanoprobes and chemosynthesis are designed specifically for constructing on the nanometer scale. Mechanosynthesis is fabrication conducted atom by atom or molecule by molecule, using small mechanical systems–e.g., nanoprobes–to control chemical reactions at specific sites [88]. Nanoprobes, such as scanning tunneling microscopes, for manipulating and imaging matter on the molecular and atomic scale are being miniaturized and refined to an incredible degree to allow deliberate and controlled manipulations of matter [18,155,202,285]. Miniaturized STMs now can be shrunk to a few tens of microns [323,324]. Visionaries, such as Drexler [88,89], suggest that someday mechanosynthesis might be refined to the extent that robotic devices the size of only a large molecule can assemble other structures atom by atom.

By contrast, chemosynthesis takes advantage of the driving force and speed of bulk chemical processes to make nanometer-scale structures. Structures manufactured by this method would have the advantage of being produced in great quantities. The fabrication of chemically-manufactured molecular switches [7,46,80,301,302], nanowires [53,54,148,254,267,321], and self-assembled monolayers [80,120,298,299,317,318] already has been demonstrated using the techniques of chemical synthesis.

Without the proper "tools" for fabrication, it is unlikely that a theoretically well-designed nanocomputer could be constructed. New research to refine the aforementioned methods of fabrication should improve our ability to manufacture reliably and efficiently on the nanometer scale. However, one great technical obsta-

cle is the problem of how to arrange enormous numbers–between 10^9 and 10^{12}–of individual devices ultra-densely and ultra-precisely on a surface or in a lattice structure. It seems highly unlikely that photolithography will be the best method for patterning such structures on the nanometer scale [233]. The recent developments in chemical self-assembly and in constructing arrays of micro-STMs establish a basis for precisely controlling and manipulating matter on the atomic level. Nevertheless, it seems nanocomputers will need to be able to compensate for small defects in their construction.

Research advances should continue to refine the aforementioned methods of nanofabrication and to expand the repetoire of nanometer-scale electronic devices that can be manufactured reliably and efficiently. These nanofabrication technologies as well as some of the advantages and disadvantages of each are examined in this section.

A. Traditional Methods of Fabrication

On the microscale, the semiconductor industry already has built the infrastructure for manufacturing computers reliably. The in-depth understanding and widespread use of lithography and molecular beam epitaxy in the microelectronics industry [55] make them good candidates for refinement to manufacture devices on the nanometer scale. However, there are some physical limitations that may prevent those methods from being the techniques of choice for fabricating future nanocomputers.

1. UV Lithography

Modern integrated circuits are produced by photolithography [284]. Photolithography is a process that beams visible or ultraviolet (UV) light through a reusable mask and onto a thin coating of photosensitive material covering a silicon wafer. This photosensitive material normally is impervious to acid, but it is degraded by the light. In subsequent steps, when the wafer is washed with acid, only the exposed areas of the silicon are removed.

To achieve the smaller feature sizes required by modern integrated circuits, lithography with visible light has been replaced by a process that uses UV light. Because of its shorter wavelengths, UV light permits greater precision. UV exposure lasts a few seconds and covers about 1 cm^2 of wafer. Therefore, an 8 inch wafer (the current industry standard) takes about an hour to expose. The limitation on UV lithography is that it only can produce features on a wafer as small as the wavelength of the UV light (about 250 nm to 350 nm in most cases.) This is approximately the feature size on conventional 256 kilobit computer memory chips. The primary advantage of such UV lithography is speed–a large area and many chips can be exposed at one time.

2. X-ray Lithography

X-ray lithography is a further refinement of lithographic techniques using ultraviolet light. This refinement provides a more precise "tool" with which to carve out a pattern on a substrate. The smaller wavelengths of X-rays allow feature sizes from 500 to 30 nm to be attained [279]. Like UV lithography, X-ray lithography uses photoresists to protect the substrate from erroneous etching. Because of the high energy of the X-rays, thicker physical masks must be used. Such masks are necessary, since X-rays are absorbed strongly by all matter, and they tend to ionize atoms in the substrate. In fact, only 2 narrow frequency ranges are available for both the "clear" and "opaque" regions of the mask. One advantage of using this technique is that it can "write" in large areas comparable to those for UV lithography. However, the high energies of the X-rays increase chances of substrate damage, and a strong source of X-rays, such as a synchrotron accelerator, is required. Such sources are extremely expensive [284].

3. Electron-beam Lithography

Electron-beam, or e-beam, lithography replaces the light beam and masks used in photolithography with a directed beam of electrons [55,119]. E-beam lithography works well for high resolution features because electrons have much shorter wavelengths than light and can be focused very precisely using electric fields. Advanced e-beam techniques can produce features down to a few tens of nanometers [145,208,255]. E-beam lithography writes like an exceedingly fine stylus since a computer controls the location of the beam with electrostatic lenses. However, such precisely focused beams also tend to cause damage from the collisions of the high-energy electrons with the substrate. Such damage lowers the conductivity of wires and, consequently, the speed of the computer. To reduce damage from the electron beam, the current can be turned down, but this increases image noise, making the beam more difficult to focus [145].

4. Molecular Beam Epitaxy

An advanced fabrication technique for creating layered surfaces is molecular beam epitaxy (MBE) [55,61]. MBE uses a beam of molecules under low pressure that collides with a heated single-crystal surface to create epitaxial layers of molecules [235]. The beam can consist of single elements or of mixtures of atoms or molecules. This technique is tailored towards building up layers of predetermined depths on a surface, but does not allow for the manipulation of the molecules in the beam to form a particular structure. Therefore, while MBE is well suited to creating microscale transistors and lasers,

it lacks the precision necessary to create nanometer-scale structures. However, the technique of chemical vapor deposition developed from MBE can be implemented in creating nanostructures using a nanoprobe and a gas over a substrate [212].

Another technology that is developing from MBE and conventional techniques for photolithography is atom lithography. Atom lithography actually "writes" the atoms directly onto the substrate. Atom lithography uses standing waves of light as a mask to guide a beam of atoms to desired resting places on the surface of a wafer [266]. This lithographic technique remains in its infancy due, in part, to the exceedingly high cost of research in these areas. There is also a reluctance of UV lithographers to change familiar, reliable UV lithography techniques for less thoroughly tested approaches [284]. These difficulties also afflict some of the even newer, emerging technologies for nanofabrication discussed below.

B. Emerging Fabrication Technologies

The limits on lithographic techniques, as well as some technological advances in other fields, have led to the consideration of some radically different approaches to achieve the extreme accuracy and precision needed to fabricate nanometer-scale electronics. These new techniques, mechanosynthesis with nanoprobes and chemosynthesis, approach fabrication from the "bottom-up". They would fabricate nanodevices by the arrangement of subunits to create a whole, rather than by removing the unnecessary parts of the starting material to leave behind the device, as is done in the traditional method of photolithography.

1. Mechanosynthesis

The mechanosynthetic or "molecular engineering" route proposes using atomic or molecular manipulators to assemble devices by positioning their atoms or molecules in the correct places one at a time or several at a time. This approach, which has been championed by Drexler [88], Merkle [219], and their collaborators, is very much in the spirit of the original concept for what has come to be called nanotechnology, as Feynman articulated it in 1959 [104]. In recent years, it is the invention of the scanning tunneling microscope (STM) [41,42] and other nanoprobes [130,241] that have suggested that the mechanosynthetic approach may become useful in the foreseeable future as a tool for "molecular manufacturing" via mechanosynthesis [18,277].

In addition to their uses in imaging and studying an atomic surface [322], STMs can be used to manipulate atoms on that surface to assemble devices. An STM employs a very sharp tungsten tip on the end of a metal foil cantilever several centimeters in length, through which a few tenths of a volt pass to a conducting sample [236]. An STM can detect or "see" atoms when the tip is in close proximity (0.5 nm) to the surface of the sample because a current is created by low energy electrons tunneling between the tip and atoms in the sample. This tunneling current changes by an order of magnitude for every 0.1 nm that the gap between the tip and the sample changes. This sensitivity translates to high accuracy and precision when "observing" features on the surface of a nanometer-scale sample.

To move an atom under the tip of an STM, the tip voltage can be increased from an "observation" voltage of approximately 0.1 volt to a "sliding" voltage of approximately 1 volt, provided the atom has little affinity for the surface [285]. If the atom one wishes to move is covalently bonded to the surface, the STM could break it loose [126,204]. However, once an atom is positioned and released by the tip, thermal energy could allow it to migrate, destroying any nanostructure being built on the surface [319]. A good example of an early, prototypical mechanosynthetic effort is the use of an STM to make the letters "IBM" with atoms individually positioned by Eigler's research group [93,285]. That IBM group was able to create the atomic "IBM" logo with inert Xe atoms on an atomically flat Ni surface, but only at cryogenic temperatures. This extremely cold environment was used, in part, to prevent migration of the atoms.

Eigler's group at IBM progressed to building a true nanoelectronic device [92] similar to the atom relay. The IBM researchers coaxed a Xe atom into switching between a Ni surface and the STM tip. (See Figure 21.) In monitoring the tunneling current, they observed current-voltage curves characteristic of microscopic transistors. More recently, a research team at IBM's Zurich Research Laboratory succeeded in moving and positioning individual molecules on a substrate at *room temperature* [155].

The ability to manipulate matter on the atomic scale permits the creation of nanometer-scale designs and structures on a surface. The STM can create nanowires on a substrate by "dripping" atoms off of its tip. When a high voltage is placed on the tip, the current rises to a level such that material from the tip itself begins to deposit on the substrate. By moving the tip as the atoms are "dripped" onto the surface, nanometer-scale wires are produced.

Chemical vapor deposition used in conjunction with an STM also can fashion wires and resistors [212]. As electrons tunnel between the tip and substrate, they decompose organometallic gases which have been introduced into the STM apparatus. This deposits metal atoms from the gas to the substrate directly under the tip. By moving the tip across the substrate, complex wiring patterns can be drawn. This last method appears especially promising to assist with fabricating devices based on the Wada atom switch design [309] and the Xe switch demonstrated by Eigler's group [92]. Currently, nanowire fabrication

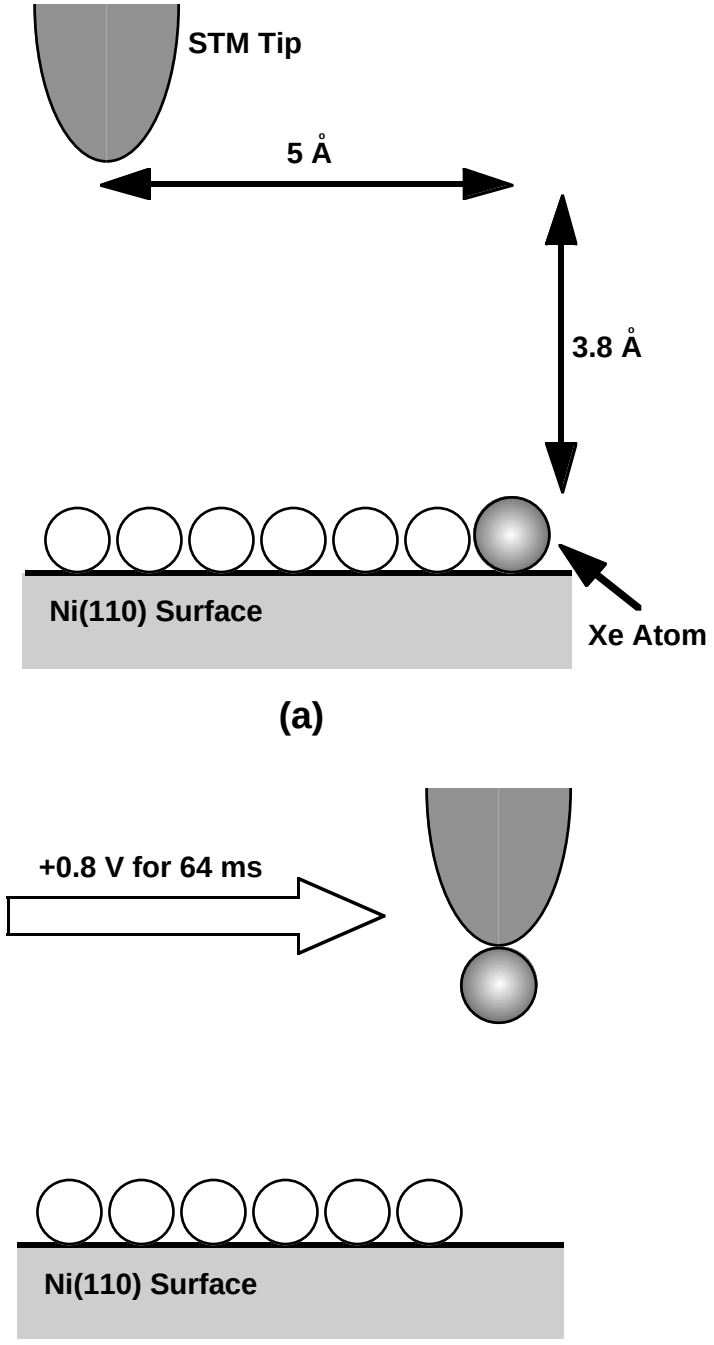

FIG. 21. Switching with an STM Tip. An STM tip can be used to create a bistable switch. There is a state of low conductance when the Xe atom is on the substrate as in (a). However, by applying a voltage and lifting the Xe atom off the surface, a high conductance state exists. Figure adapted from Eigler *et al.* 1991 [92].

appears to be the most developed area of mechanosynthesis [75,97,146,257,263,285], but work also is being done to develop nanometer-scale lithography by directly patterning a substrate using an STM [77,96,202]. The ability to assemble nanostructures rapidly and economically by mechanosynthesis is important if it is to become a practical approach for their manufacture. The preceding examples all used a single STM tip to manipulate matter into useful devices. It would be a tedious and costly process to build a computer in that manner. A first step toward multiplying the capability of the STM for the purpose of improving the efficiency of the process is the effort of MacDonald *et al.* at Cornell University towards creating an array of several hundred small, independent STM tips on a chip. The Cornell group has had success in fabricating an individual micro-STM, measuring 200 micrometers on a side [323,324]. Images of the micro-STM and its tip are shown in Figures 22 and 23.

Also essential for practical mechanosynthesis are improvements in user interfaces for nanoprobes, to make manipulating matter on the atomic scale a more natural and transparent process. A consortium of computer scientists, chemists and physicists from the University of North Carolina and the University of California at Los Angeles has created a prototype device called the "Nanomanipulator," by integrating with an STM (or AFM) an immersive virtual world interface. The Nanomanipulator allows a user both to control the nanoprobe and to "experience" the nanoscopic domain [98]. This experience presently includes being able to "feel" atoms as well as to push them across a surface with the user's hand.

With several generations of improvements in nanoprobe arrays and user control interfaces, as well as in the tip technology for nanoprobes, a successor to MacDonald's prototype micro-STM array might one day be incorporated into accessory hardware for a workstation. This could permit a kind of "desktop molecular manufacturing" via mechanosynthesis. This type of development would apply a micro-STM array like that of MacDonald to the molecular positioning being done at IBM-Zurich [155], under the control of an interface such as the UNC "Nanomanipulator" [98].

Another nanoprobe device with some similarities to the STM is the atomic force microscope (AFM) [130,236]. The AFM monitors deflection of a cantilever as it rides along a sample's surface instead of monitoring an electric current between the tip and sample. This is important because this means the sample need not be conductive. While the AFM does not offer the dexterity of an STM nor the ability to coax atoms to jump [47], it does, however, provide a unique means of "pushing" atoms and molecules around a surface regardless of their conductivity [51,125,143,178,262]. A type of nanolithography based on AFMs already is being developed [314], and 100 nm MOSFETs with 60 nm feature sizes have been constructed using AFMs [224].

Drexler has suggested that an AFM might be used with a receptor tip to "grasp" molecules made by traditional chemical methods and position them with atomic precision [88]. STMs already can be used to position atoms with stunning precision [74]. However, the assembly of structures using individual atoms and molecules placed with atomic precision still is not a routine or reliable process. Drexler's vision probably must await another generation of much more precise nanoprobes with much more selective retention of atoms at their tips.

2. Chemosynthesis

Another route emerging for fabrication of the components for nanometer-scale electronics is chemosynthesis– the bottom-up synthesis of nanostructures by chemical processes. There still are significant technical obstacles to the widespread chemical fabrication of arbitrary man-made nanostructures and nanodevices. However, research in this area is stimulated and guided by the ubiquitous involvement of chemical synthesis in the formation of all sub-microscopic biological structures and organisms. The apparent impracticality of using macroscopic or even microscopic mechanical probes to assemble huge numbers of nanoscopic structures is another stimulus to the active consideration and experimentation with chemical routes for the fabrication of nanostructures.

Chemical Self Assembly. A form of chemosynthesis that is of increasing importance is chemical self-assembly [318]. Chemical self-assembly is the spontaneous orientation of a number of molecules into an energetically favored *supra*molecular structure without human intervention. This most often occurs through noncovalent bonding among molecules. Information about the supramolecular structure is encoded in the molecular components through their shape, functional groups, etc. Although the systematic study and synthesis of such systems is a relatively new sub-discipline, significant and encouraging advances have resulted from early efforts [7,80,210,315]. The heuristics and techniques necessary for realizing the chemical self-assembly of nanostructures are being developed and refined continually [40,64,100,101,120,189,298,299,317,318].

Naturally occurring self-assembled systems of complex supramolecular structures, such as DNA, cell membranes, chromophores [173,273], or even viruses, provide models with which to refine the process of artificial chemical self-assembly. In nature, chemical self-assembly does not rely primarily upon covalent bonding to shape a nanostructure such as DNA [315]. Self-assembling molecules require weak interactions among constituent molecular subunits to produce stability. These weak interactions include hydrogen bonding, electrostatic interactions, and van der Waals forces. For example, hydrogen bonding acts in DNA to orient its small molecular subunits–nucleotides–and to hold together the interpen-

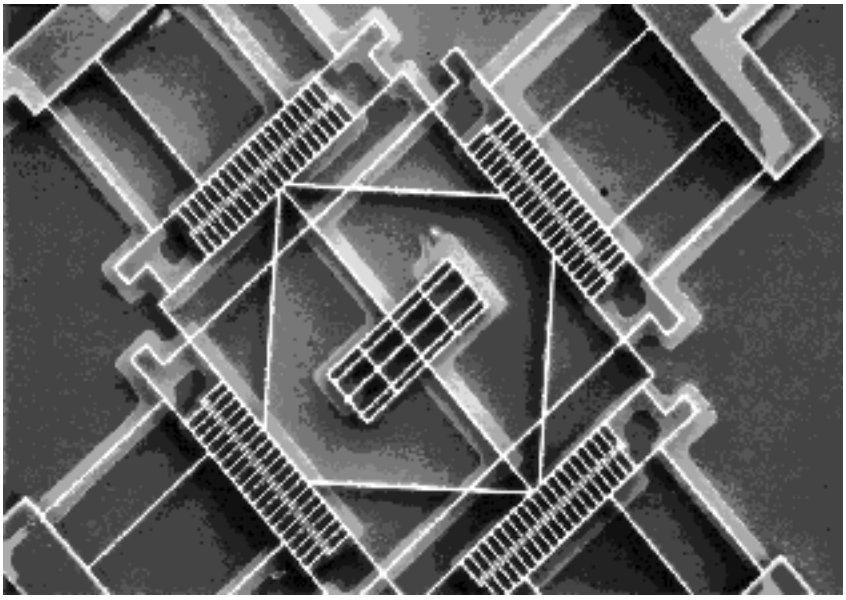

FIG. 22. SEM Micrograph of a Micro-STM. Scanning Electron Microscope (SEM) micrograph of a 200 μm by 200 μm micro-STM. Reproduced with permission of Prof. Noel MacDonald *et al.*, Cornell University [324].

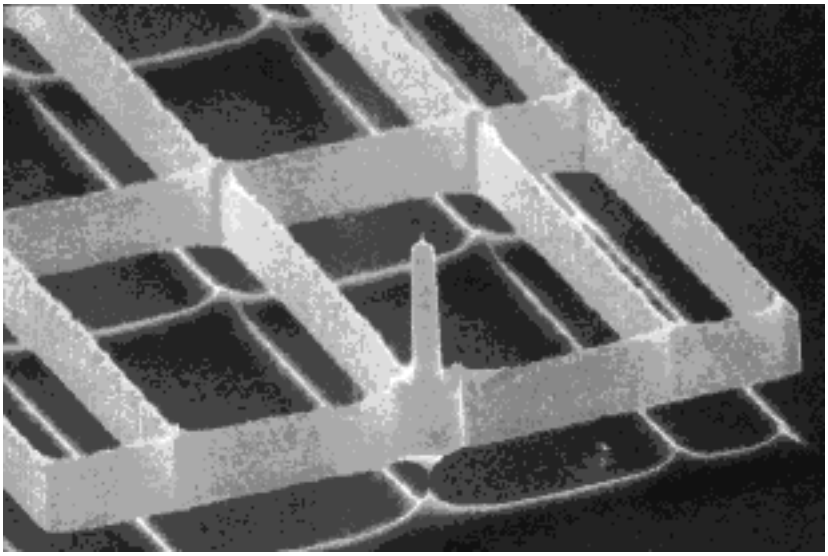

FIG. 23. SEM Micrograph of a Micro-STM Tip. SEM micrograph of individual micro-STM tip manufactured by the Cornell University group. The width of the entire structure shown is approximately 20 μm. Reproduced with permission of Prof. Noel MacDonald *et al.*, Cornell University [324].

etrating helical chains of nucleotides. (Hydrogen bonding is the weak attraction between a covalently bonded hydrogen of one molecule and an electronegative atom, such as nitrogen or oxygen on another nearby molecule.)

One important advantage of chemical self-assembly over other methods of nanometer-scale fabrication is the error-correction process inherent in the self-assembly of chemical nanostructures. As a self-assembling chemical system attempts to reach a thermodynamically stable state, it tends to rid the growing structure of any molecules of the "wrong" type or in the "wrong" position that are caught in the assembly process. This permits self-assembly processes to create very many *identical* copies of nanometer-scale structures that are particularly stable and sturdy. Massively parallel processes for the fabrication of nanostructures also are possible because of the extremely large number of identical molecular initiation points for self-assembly that are found in a typical solution. This is significant because the fabrication of many nanostructures in parallel seems imperative for the efficient production of future ultra-dense computer designs that are projected to consist of trillions of individual components.

While many methods for chemical self-assembly rely on the interaction of molecules in a solution [120,315,317], George Whitesides' research group at Harvard University is investigating an alternative approach that produces self-assembled monolayers (SAMs) on a substrate [124,167,174]. Using small organic molecules with a functional group at one end, the molecules attach to the substrate in a single layer. Several methods exist for patterning the adsorption of the molecules onto the substrate including electropolymerization and contact printing. Reifenberger *et al.* at Purdue University have adapted the SAM method to attach individual gold clusters on top of the SAM [80] by using self-assembling molecules with functional groups on both ends invented by Tour [267], as illustrated in Figure 24. As shown in Figure 25, this technique creates two-dimensional arrays of regularly spaced gold clusters. Molecular-scale circuits using such arrays of gold clusters might be fabricated in this manner. The arrays are manufactured on the nanometer scale with minimum feature sizes around 2 nm [80].

Recent experiments also have been reported in which nanometer-scale holes were punched into SAMs using tightly focused beams of energetic metastable ions [40]. Techniques such as this may permit SAMs to be "sculpted" to refine the precision and reliability with which they can be used to produce patterns on a surface. This would allow SAMs to act as resists, protecting a substrate from being etched away by acid. Recent work by Jackman and Whitesides [149] also shows the potential of using SAMs to manufacture integrated circuit components on curved surfaces. This is difficult, if not impossible, with present-day lithographic techniques because it requires multiple depths of focus for the photon beam.

Chemical Synthesis of Molecular Electronics. Much chemosynthetic research has been performed in attempting to realize a molecular switch via chemosynthesis [45], stimulated by Aviram's proposals for molecular electronics [13,15,17]. For example, James Tour's research group at the University of South Carolina has been developing conducting oligomers that are connected perpendicular to each other [267,301,302]. Structures such as the one depicted in Figure 26 are theorized to behave as switches under certain conditions [15,17]. (Oligomers are chains of repeating molecular subunits that can be linked together by extended π systems.)

Whitesides' group [20] and Tour's group [303] also have shown that thiol (-SH) functional groups adsorb well to gold surfaces and act as "alligator clips" for attaching molecular electronic units to a semiconductor substrate. Recently, Tour showed a single molecular wire inserted into a SAM to be conductive [53]. This approach is driving forward experimentation, such as the research by Mark Reed at Yale [249], to realize a molecular electronic switch. The approach could incorporate the chemical synthesis of the switch with the process of self-assembling the circuit on the gold leads. A group at Purdue University has already demonstrated a Coulomb staircase for a self-assembled nanostructure at room temperature [7]. This nanostructure incorporated oligomers of the type invented by Tour [267].

Assembling polymers directly onto a patterned substrate could furnish a new method for creating nanometer-scale computers. Whitesides' research group has demonstrated that it is possible to control the deposition of molecules on a substrate. If the molecules deposited on the substrate were molecular electronic switches, such as Tour is developing, it seems possible that they could be positioned to build a circuit. After the reaction is completed, the substrate could be washed of the unbound switches and another type of molecule introduced to connect adjacent switches together. Such a process might be used to manufacture a truly molecular-scale circuit via chemical steps. One drawback of such a technique would be the errors introduced at each step. These errors would compound with each step. Thus, for example, in an extreme case to illustrate the point, a 25-step process, where 90 percent of the molecules attach correctly to the substrate in any given step, would yield a completed structure where only 7 percent of the electronic devices would be connected properly.

Hybrid Chemosynthetic Methods. A particularly promising development in nanolithography is the recent success of a hybrid approach that combines the use of atom beams with some of the techniques of self-assembly. A beam of atoms has the potential to be a very precise tool for etching a monolayer or surface, because the large mass and momentum of the atoms makes its quantum wavelengths very short (approximately 0.01 nanometers). A Harvard University team, under the leadership of Professors Mara Prentiss and George Whitesides, used a beam of excited argon atoms to put a pattern of holes

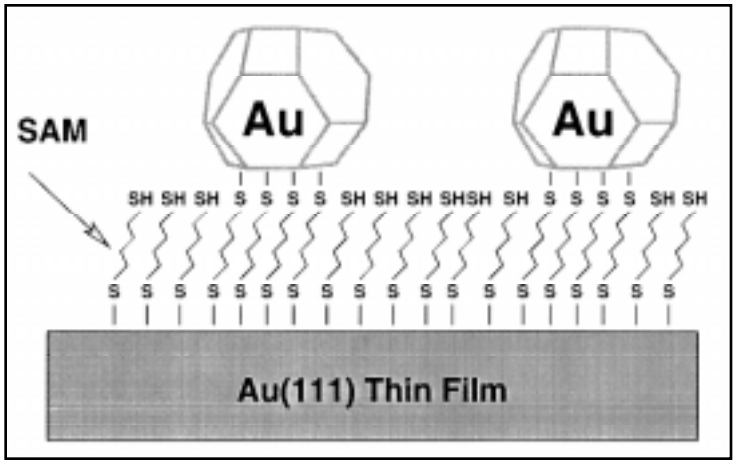

FIG. 24. Side View of a Self-Assembled Array of Gold Clusters with Molecular Electronic Properties. Schematic side view of gold clusters 5 nm in diameter attached to a SAM by molecular wires. Figure courtesy Prof. R. Reifenberger, Purdue University.

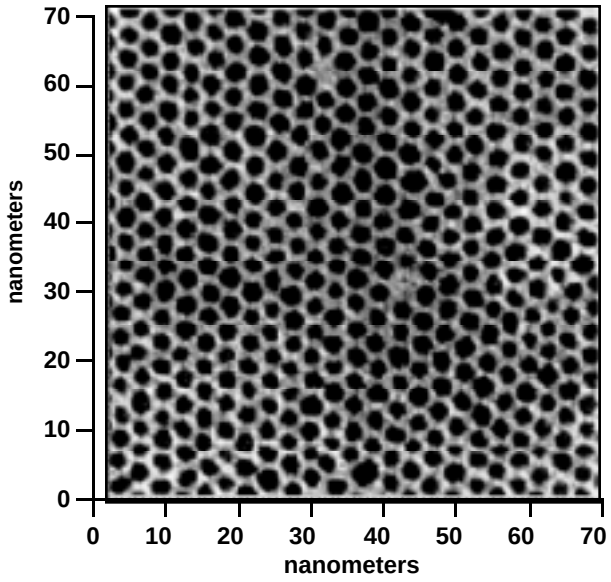

FIG. 25. Top View of a Self-Assembled Array of Gold Clusters with Molecular Electronic Properties. In the scanning electron micrograph, each dark dot represents a gold cluster 2-5 nm in diameter. Figure courtesy Prof. R. Reifenberger, Purdue University.

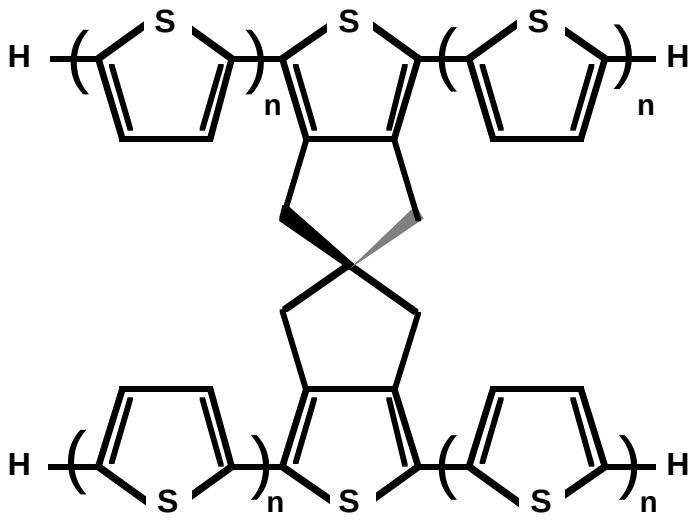

FIG. 26. Aviram's Proposed Spiro Switch. The two oligomer wires are joined perpendicular to each other by an sp^3-hybridized carbon atom bridge.

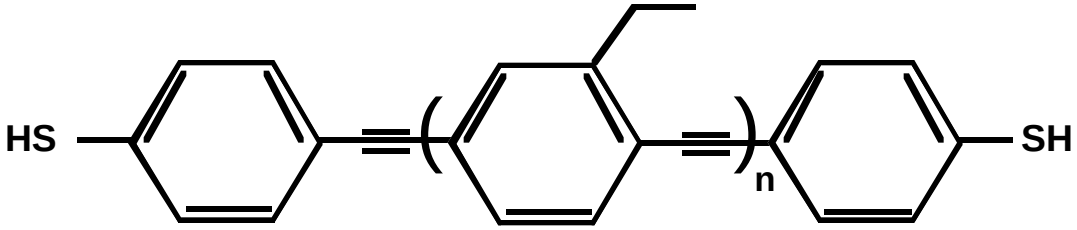

FIG. 27. Conducting Molecular Wire synthesized by Prof. James Tour *et al.* [53]. The two thiol groups on the ends act as molecular "alligator clips" for connecting the wire to metal electrodes on either side.

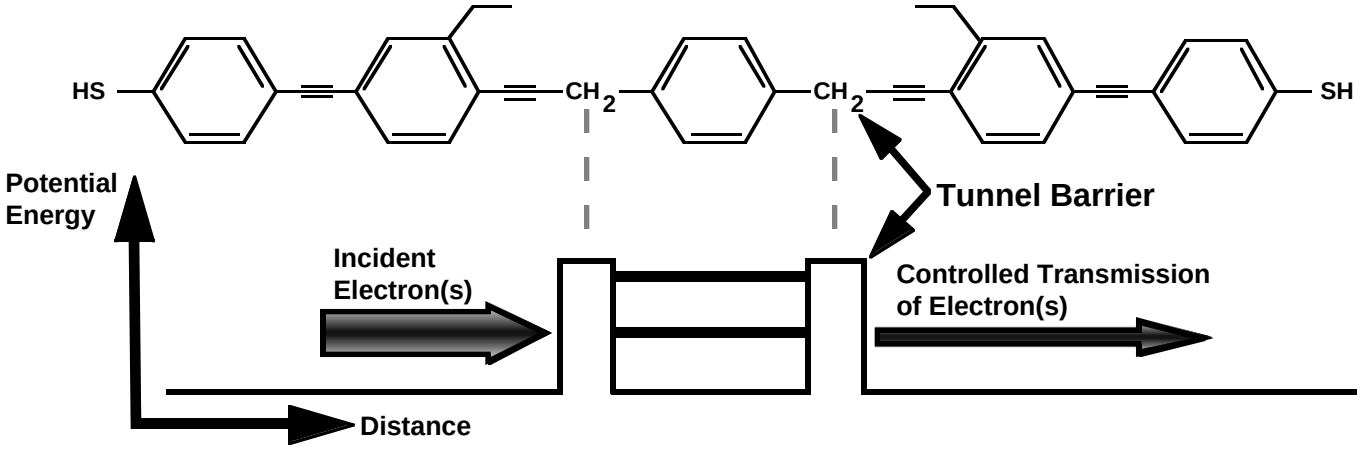

FIG. 28. Molecular Quantum-Effect Device. Using the basic chemical components of the wire shown in Figure 27, it is possible to create other useful molecular electronic structures. The molecule shown here has an embedded potential well (shown schematically beneath the structure diagram) that should allow the molecule to behave in a manner analogous to solid-state RTDs made from semiconductors [304], as depicted in Figure 3.

in a monolayer resist that had been self-assembled on the gold surface [40]. Then, the surface was etched in the holes with a ferricyanide solution to shape gold features on the silicon substrate. In the initial experiments, the resolution of the lithography was finer than 100 nanometers, and the Harvard group asserts that the technique has the potential to inscribe features on a surface with at least 10 nanometer resolution.

Chemically-Created Nanowires. Chemosynthesis, like mechanosynthesis, also has been successful in fabricating nanowires. Bein and co-workers [321] use mesoporous host structures [30] as templates to create carbon-based conducting polymer wires 3 nm in diameter. A similar method developed by Martin and co-workers [54] also polymerizes wires inside of small channels. These nanowires show high conductivity compared to bulk polymers, suggesting a coherent (wire) structure. Tour and his collaborators [53,303] have more recently shown other potential molecular wires that could be self-assembled onto a gold surface.

Another new type of nanostructure, termed a "buckytube" because of its structural similarity to carbon "buckyballs," also presents possibilities for chemically synthesizing nanowires [148,254]. Buckytubes and buckyballs are examples of a class of chemically synthesized molecular nanostructures known as buckminsterfullerenes [83]. Buckytubes are cylindrical carbon nanotubes. It is anticipated that these hollow tubes might be filled with conducting metal atoms to create among the strongest structural nanowires chemically possible. The structure of the nanotube derives its strength from the carbon-carbon bonds. The carbon atoms are bonded in hexagonal arrays, and these arrays are arranged so that virtually no flaws exist in the structure. A study of the molecular dynamics of the carbon nanotubes has shown that isolated flaws in the structure migrate to the ends of the tube and are eliminated by the rearrangement of individual covalent bonds. This observation has suggested to some investigators that carbon nanotubes are "self-healing" [49]. A measurement of the conductivity of carbon nanotubes has shown that a 10 nm tube can carry currents of approximately 10 microamps per fiber [316]. More recent work by two research teams show that, in theory, carbon nanotubes could be made to behave like electronic switches [276]. The aforementioned circuit array self-assembled by the Purdue University group [7,80] also represents a significant step in the chemosynthesis of structured nanocircuits.

However, as discussed at the beginning of this article, the essence of electronic computation is switching with two-state or multi-state devices in precisely arranged circuits or logic structures. Therefore, to chemosynthesize or self-assemble a nanometer-scale electronic computer, one must be able to use these methods to fabricate prescribed arrangements of such switching devices. A large step in this direction appears to have been taken recently by Mallouk and his collaborators at Penn State University. They report the chemical self-assembly of a functioning SET [100,101].

Despite such significant advances in the chemosynthetic self-assembly of simple structures that should be useful in nanoscopic electrical circuits, the chemosynthesis or chemical self-assembly of entire computers, or even small logic elements, appears to be beyond the present state of the art. To attain this goal, it is likely that there must be much further refinement of empirically grounded heuristic guidance for the invention and application of practical chemical self-assembly techniques. Only the first, basic steps have been taken in this direction. One may anticipate that these steps might lead, eventually, to a more comprehensive framework of heuristic and theoretical insights upon which to base experimental and industrial application of chemical synthesis for the fabrication of nanocomputers.

VII. EMERGING TECHNOLOGIES FOR THE IMPLEMENTATION OF NANOELECTRONICS

All of the preceding developments toward nanometer-scale quantum-effect electronic devices are very promising. However, significant obstacles are that (1) most such devices are difficult to fabricate reliably and efficiently, plus (2) they operate only at cryogenic temperatures. In order for proposed devices such as SETs and quantum dots to operate at room temperature, they must be small. This is because the switching states must be separated in energy by an amount greater than the energy kT of the ambient background thermal "noise" (where k is Boltzmann's constant and T is the absolute temperature). Quantum mechanics dictates that the energy levels get farther apart within a very small structure for electron confinement–e.g., a quantum dot–as the spatial dimensions of the structure get smaller. For structures with dimensions of 10 nm or less, it is predicted that the energetic separations between the switching states should be greater than the thermal background energy at room temperature. Two routes that have been discussed widely for overcoming these obstacles are molecular electronics and, in the solid-state, silicon nanoelectronics. Both routes show promise for allowing operation of nanocomputers at room temperature. Also, silicon nanoelectronics can take advantage of the electronics knowledge and experience already gathered by the semiconductor industry.

A. Molecular Electronics

The inorganic chemistry of solid silicon surfaces governs the fabrication and implementation of present-day microelectronics. However, there presently is much research focused on using the greater power and variety of organic chemistry to create molecular-scale electronic

devices [16,45,58,59,140,232]. This approach should offer more options for designing and fabricating nanometer-scale devices than presently is available for producing solid-state chips with nanometer-scale feature sizes. Molecular electronics uses primarily covalently bonded molecular structures whose function involves discrete molecules, separate from an extended solid. (This is distinguished from organic microscale transistors and other such organic semiconductor-like circuits that use bulk materials and bulk-effect electron transport.)

The advantage of using single molecules to form wires and quantum confinement structures from which to assemble an electronic computational device is that molecules inherently are nanometer-scale structures. Therefore, it seems probable that switches made using quantum confinement structures within molecules can be made to operate at room temperature. Also, molecular structures often can be made in large numbers reliably and with great uniformity. Thus, the fabrication technique of chemical self-assembly discussed above in Section VI B 2 is likely to be a key method with which to build molecular electronic computational systems from large numbers of nanometer-scale quantum devices.

In order to realize molecular electronics, three obstacles must be overcome. First, molecules must be made that exhibit the requisite electronic effects, such as Coulomb blockade. Second, there must be a method for arranging and linking molecules, using intermolecular bonding, into patterns corresponding to useful computational devices. Third, there must be a way to connect the resulting supramolecular devices onto a pre-formed two-dimensional solid substrate or into a three-dimensional matrix with the correct placement of the parts [13,17].

The search for individual molecules that would behave as switches began with a theory on molecular rectification proposed by Ari Aviram and Mark Ratner in 1974 [13]. Research on molecular electronics was stimulated in the early 1980s by a few key investigators and the efforts of such visionaries as the late Forrest Carter [58,59]. However, it was the invention of the STM in 1981 [41,42], providing a means to manipulate and image individual atoms and molecules, that contributed much of the impetus to the extensive research on molecular electronics today [7,53,80,152,172,194,227,267,301–303].

In 1988, the discipline was again furthered by Aviram's proposal of a more developed theory for molecular electronics. The refined theory included a potential molecular switch design, the spiro switch [15]. Also, Hopfield, Onuchie, and Beratan proposed a molecular shift register to be used for molecular electronic memories [10,142]. Motivated by the work of Aviram, James Tour began synthesizing a few spiro switch-like molecules in 1990 [267,301,302], while Martin *et al.* demonstrated molecular rectification using a Langmuir-Blodgett film [209,261] based on Aviram and Ratner's theory. More recently, several research groups, including one at Purdue University [7,80], have demonstrated Coulomb blockade and Coulomb "staircases" with molecular nanostructures at room temperature. Also, Tour, Allara, and Weiss have demonstrated conductance through a *single* molecular wire [53]. (The structure of this molecular wire is shown in Figure 27.) There also have been a number of recent efforts towards modeling the conductance through single molecules [151,153,225–227,260].

Mark Reed at Yale University is measuring the conductance of individual molecules, such as those designed and synthesized by Tour, in hopes of finding a suitable molecular structure for a molecular transistor [250]. In very recently reported experimental results, it appears that these efforts by Reed, in collaboration with Tour, may have produced measurements of *individual molecules* that act as quantum-effect devices [251]. In the Tour, Allara, and Weiss experiment [53] showing conductance in a molecular wire, one end of the conducting molecule is adsorbed to a gold surface, but an STM tip is used as the other electrode in the circuit. However, in the more recent work by Reed and Tour, each end of a conducting molecule is adsorbed to a different gold electrode mounted on a surface in order to complete a circuit.

Individual switches such as the spiro switch [15] and nanostructures demonstrating Coulomb blockade [7,80,251] have been fabricated. Other very significant advances are Tour's demonstration of conductance through a single molecular wire [53], the development of a technique for systematically lengthening potential wires [267], the Purdue group's fabrication and demonstration of arrays of nanostructures with molecular electronic properties [7,80], as well as the recent Reed-Tour report of a molecular quantum-effect device [251]. Further development upon molecular wires, like those synthesized by Tour, may allow the implementation of tunnel barriers like those shown schematically in Figure 28, or other features necessary for creating a useful two-state or multi-state device [304].

Despite these significant advances toward the development of practically applicable molecular quantum-effect wires and switches, molecular three- and four-terminal devices, gates, and logic arrays need to be designed, fabricated, and demonstrated before an effective molecular CPU or memory device is possible. The problem of how to connect molecular components to each other in order to construct logic has yet to be addressed outside of theory. Tour has suggested that it may be necessary to re-think electronic computer designs and architectures in order to make the most effective use of the properties of molecular electronic devices [304]. Simply using them to mimic the designs suitable for much larger and less uniform solid-state devices with vastly different behaviors may not be the most advantageous approach. Notably, a conventional, solid-state digital circuit contains only 10^9 or 10^{10} individual two-state devices per square *centimeter*, while it is easily possible to fit 10^{13} or 10^{14} two-state molecular devices into a square *millimeter*. This is a potential increase in device density by a factor of as much as 10^7–i.e., 10 million! This fact, alone, should stimulate new thinking.

The issues mentioned above are among the many technical obstacles that remain on the path to creating molecular electronic computational devices. Among the other challenges to fulfilling the vision of Aviram, Ratner, Carter, and their disciples are:

- Development of a more comprehensive theory of electron flow through individual molecules
- A generalized method for connecting synthesized molecular switches and wires into circuits
- A refined understanding of the heuristics of self-assembly

The cost of research in order to overcome these challenges and to realize a molecular electronic computational device may be high. However, the potential advantages from a pursuit of molecular electronics include a vast reduction in the cost per bit, a vast increase in bit density, a decrease in cycle time, a reduction of energy per bit cycle, and, possibly, three-dimensional ultra-densely integrated computational systems [10]. In a single chemical reaction on a desktop, it should be possible to synthesize approximately 10^{23} two-state devices all at once [304]. This is many more devices than exist in all the computers presently in use in the world today. For this reason, as well as a those discussed at the beginning of this section, it seems likely that molecular electronics will be the ultimate solution to the problem of the economical fabrication of ultra-dense, nanometer-scale computer electronics.

B. Silicon Nanoelectronics

Another alternative to implementing quantum-effect electronics on a nanometer scale is through the use of silicon (Si). Microelectronic transistors with feature sizes less than a micron and RTDs developed to date are manufactured using pairs of III/V metals such as GaAs [114,312]. However, the possibility of silicon-based nanoelectronics is enticing to the semiconductor industry. Silicon *nano*electronics would draw on the industry's knowledge base in planar IC manufacturing gathered from the manufacture of silicon-based *micro*electronics. Si also offers two important technical advantages over GaAs and other III/V compounds in that (1) Si has a lower thermal conduction limit, and (2) while electrons move faster in GaAs than in Si in low electric fields, both materials behave similarly in high fields [214,215]. Also, manufacturing techniques could allow more reliability and uniformity in the processing of silicon substrates than is possible with doped III/V alloys. The use of silicon rather than III/V semiconductors should be more economical over time and ecologically safer for the environment. (Production of GaAs and other III/V compounds generates arsenic and other poisonous by-products.)

Much research is being performed to create nanostructures using Group IV and silicon alloys such as silicon germanium [23], in an effort to reduce feature sizes to below 0.1 micrometers. An ongoing effort at Texas Instruments led by John Randall and Alan Seabaugh is attempting to incorporate RTDs into silicon oxide transistors to create high-density memory devices. It is projected that a high-density static random access memory (SRAM) with 1 bit/square micrometer is possible using high temperature submicrometer Si-RTDs [246]. Steven Chou at the University of Minnesota actually has constructed single-electron and single-hole quantum dot transistors in Si [63,187]. These are only some of numerous efforts in progress to realize silicon-based nanoelectronics.

However, to date, a nanometer-scale quantum heterojunction made out of silicon has not yet been demonstrated. A heterojunction is necessary to create a potential well or barrier, the basis for constructing a solid-state quantum-effect device, such as a resonant-tunneling diode or resonant-tunneling transistor. Tunnel barriers or heterolayers also will be needed to control leakage current in a nanometer-scale silicon-based device. When such issues are resolved, it is likely that Si-based nanoelectronics will begin to supplement or perhaps replace the use of III/V compounds in electronic devices.

VIII. MODELING

Details of the form and behavior of nanometer-scale structures are dependent upon quantum mechanical effects that can be small and subtle. Thus, quantum mechanical modeling of potential nanoelectronic devices and structures will become increasingly important for their design and implementation. Computational modeling should provide a better understanding of the parameters and constraints for these nanoelectronic devices and create a framework for interpreting experiments. Modeling may even reduce the need for costly experimentation. Conceivably, modeling also could give new information about nanodevices that is not evident through experimentation alone.

Since the hard-to-solve Schrödinger equation governs the behavior of all quantum mechanical systems, modeling them requires finding approximate solutions of this differential equation. There are three major classes of systems for which the Schrödinger equation must be solved in order to model most nanoelectronic devices. One class is solid-state electronic devices in which there is a "sea" of valence electrons that move through the system nearly ballistically, and which may be treated approximately as plane waves. The second is molecular electronic devices where the wave functions die away exponentially.

A third, more complex class of system for modeling, a mixed solid-state/molecular device such as the one being developed by Reifenberger and his collabo-

rators at Purdue University [7], has arisen due to advances in nanotechnology. Such mixed structures utilize both solid-state metal devices and molecular wires. As current passes through the molecular wires, it is necessary to model the molecular system using both plane waves approximating the electrons moving through ballistically and exponential functions to represent the more tightly bound electrons. There is much recent research on modeling the conductance of single molecules across two metal contacts [151,153,225–227,260].

Three-dimensional, computer-intensive modeling will be needed for describing systems of molecular wires and quantum dots [127]. In the late 1980s and early 1990s, Mark Reed, William Frensley and James Luscombe of Texas Instruments described the need for understanding the dynamic behavior of resonant-tunneling devices [115,200,201,247]. In 1992, Lent described simple models of the local Coulomb-effect interactions of two electrons confined in semiconductor quantum dots using a two-particle Schrödinger equation [179]. This contributed to the formulation of the Lent-Porod cellular automata design.

Presently, there are a number of efforts worldwide to improve device modeling. IBM, AT&T, NEC, Hitachi, and others are working towards the goal of a fully three-dimensional modeling system with an incorporated Schrödinger solver for quantum devices [103]. The U.S. Government is providing funding for the NEMO (Nanoelectronic Modeling) program to develop a standard, easy-to-use software capability to model the properties and behavior of solid-state nanoelectronic devices. David Ferry of Arizona State University is developing the numerical modeling of quantum dots [2,103].

Electron-density-based modeling approaches, "density-functional theories" [237,313], and their refinements also are beginning to be applied to model nanoelectronic devices [95,147]. These methods show promise for their mathematical and conceptual simplicity, as well as for their potential computational speed.

IX. REMAINING CHALLENGES FOR NANOELECTRONICS

Recent research advances provide great hope for the future of electronic nanocomputing. A number of nanometer-scale devices have been fabricated and demonstrated. The capability to fabricate arrays of nanometer-scale structures also has been demonstrated, as have innovative combinations of devices and arrays. However, the capability does not exist yet to build logic structures or computers from nanometer-scale components. Furthermore, almost no attention has been devoted yet to devising and putting in place the infrastructure for manufacturing thousands or millions of such ultra-large-scale integrated (ULSI) computers. Many challenges and technical obstacles remain.

The first set of challenges lies in the design and implementation of the nanometer-scale devices themselves. The foremost of these challenges is to raise the operational temperatures close to room temperature. The reliable, precision manufacture of many such devices is yet another challenge. The development of a molecular two-state device or silicon nanoelectronic device could provide a way to meet these challenges.

However, the greatest challenges for nanoelectronics may lie after the realization of a reliable two-state or multi-state device. Before building a computer from such devices, a functioning logic structure such as a gate must be demonstrated. The devices must be arranged and connected densely in units that can perform basic logical and arithmetic operations. Architectures also must be devised for organizing the dense logical and arithmetic units on a still broader scale to make an efficient computer. Processes for error correction must be invented that can be incorporated as an intrinsic feature of whatever designs and architectures are used to organize billions or trillions of ultra-small, sensitive electronic devices. Finally, a very formidable challenge awaits in the conversion of research on small numbers of prototype nanodevices and nanocomputers to practical and reliable mass-produced systems.

At the highest level of consideration for the emerging technology for nanocomputing is the likely requirement for the interaction of nanoelectronics with microelectronics. It may be envisioned that nanoelectronics might someday replace microelectronics. However, in the short term, it is likely that nanoelectronics must be integrated into conventional microelectronic designs. Then, in the long term, scientists and engineers working in the field of nanoelectronics also can strive towards a general purpose ULSI computing engine with simple interfaces.

X. CONCLUSION

There is a growing awareness in the microelectronics community that conventional bulk semiconductor technology and photographic etching techniques are nearing their theoretical and economic limits for the production of more densely integrated and faster electronic computers. New approaches to building computers are necessary to ensure continued technical progress at the current rate. Yet it seems unwise to abandon almost 50 years of experience with electronic computation based on two-state logic devices. The answer might lie with nanometer-scale electronic devices that build upon experience with microelectronics, but take advantage of the very same quantum effects that limit current micro-scale transistors. Practically applicable resonant-tunneling devices, quantum dots, or single-electron transistors should be attainable with next-generation technology. The ongoing revolution in miniaturization–fabrication on the micron and nanometer scale–should assist in the transition to

solid-state nanoelectronics. However, smaller molecular electronic devices are likely to require further research before they become usable in functioning, practical electronic computers. The ultimate choice of technologies and designs for electronic nanocomputers will depend on a number of factors including device speed, power dissipation, reliability, and ease of fabrication.

Based on the research discussed in this article, it seems likely that the first practical nanoelectronic circuits will emerge from the laboratory a few years after the beginning of the 21st century, as suggested in Figure 6. These solid-state ULSI circuits are likely to employ "hybrid" devices, such as resonant-tunneling transistors, combining nanometer-scale structures that rely on quantum effects along with conventional bulk-effect microelectronic transistors [57,246]. This should permit the development of terabyte memory chips [307,308] and experimentation with novel massively-parallel processor architectures. Such circuitry may undergo evolution to achieve even more dense, reliable solid-state structures with feature sizes as small as 10 nanometers. These might be manufactured using atom beam lithography, self-assembling masks, and other emerging fabrication technologies. Such second-generation ULSI circuits probably will be made from silicon-based compounds, although present solid-state quantum-effect devices are made almost exclusively from III/V compounds, such as gallium-arsenide. Ultimately, however, molecular electronics will be necessary to achieve reliable, high-temperature operation and ease of fabrication for quantum-effect circuitry with nanometer-scale components. The first steps have been taken in this direction [7,53]. With a few more early advances, developments in molecular electronics may even race ahead of those in solid-state nanoelectronics.

No matter how an electronic nanocomputer is implemented, research on nanotechnology is providing investigators with increasingly sensitive, accurate, and robust tools for molecular-scale manipulation. It is likely that soon it will be possible to "read" and "write" matter as easily as we read and write information on magnetic computer disks. As a consequence, the line between hardware and software will blur. Should the new arrays of STMs built upon computer chips become as easy to produce as modern CPUs, it might be possible for the end user to design and build his or her own nanoelectronic computers. These might be application-specific devices that could be discarded, like data, at the end of a computation, with the matter (atoms and molecules) in them being reused to write the next computer. In the future, matter will be software.

Nanocomputers will arrive as a result of breakthroughs on many fronts. The excitement of standing on the threshold of such an innovation is enhanced by the multidisciplinary nature of nanotechnology. It is impossible to predict from which traditional discipline will come the impetus or key breakthrough necessary to construct these new, much tinier computers with much greater speed and power. One only can be confident that such dramatically smaller computational engines, along with the methods devised to fabricate them, will transform electronic computing and our technological infrastructure, as well.

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XIII. BIBLIOGRAPHY

[1] Adleman, L., "Molecular Computation of Solutions to Combinatorial Problems," *Science*, Vol. 266, 11 November 1994, pp. 1021-1023.

[2] Akis, R., and Ferry, D. K., "Numerical Modeling of Quantum Dot Structures," This paper is available on the Internet World-Wide Web at the following URL: http://enuxsa.eas.asu.edu/~akis/report.html

[3] Allinger, N. L., Yuh, Y. H., and Lii, J. H., "Molecular Mechanics. The MM3 Force Field for Hydrocarbons 1," *J. Am. Chem. Soc.*, Vol. 111, 1989, pp. 8551-8566. See also references cited therein.

[4] Amabilino, D. B., and Stoddart, J. F., "Interlocked and Intertwined Structures and Superstructures," *Chem. Revs.*, Vol. 95, 1995, pp. 2725-2828.

[5] Anantram, M. P., and Roychowdhury, V. P., "Can Metastable States Affect Ground State Computing?" *Proceedings for the PhysComp96 Conference*, Boston, MA, November 22-24, 1996.

[6] Ancona, M. G., "Design of Computationally Useful Single-Electron Digital Circuits," *J. Appl. Phys.*, Vol. 78, 1995, pp. 1-14.

[7] Andres, R. P., *et al.*, "'Coulomb Staircase' at Room Temperature in a Self-Assembled Molecular Nanostructure," *Science*, Vol. 272, 31 May 1996, pp. 1323-1325.

[8] Anelli, P. L., *et al.*, "Molecular Meccano 1. [2]Rotaxanes and a [2]Catenane Made to Order," *J. Am. Chem. Soc.*, Vol. 114, 1992, pp. 193-218.

[9] Angell, J. B., Terry, S. C., and Barth, P. W., "Silicon Micromechanical Devices," *Scientific American*, April 1983, p. 44.

[10] Ashton, G., ed., *Solid-State Memory Study*, National Media Lab, 1994. This study is available on the Internet World-Wide Web at the following URL: http://www.nml.org/publications/NML_TR /solid_state_memory_study/toc.html

[11] Atkins, P. W., *Molecular Quantum Mechanics*, Second edition, Oxford U. Press, Oxford, U.K., 1988.

[12] Atkins, P. W., *Quanta: A Handbook of Concepts*, Second edition, Oxford U. Press, Oxford, U.K., 1992.

[13] Aviram, A., and Ratner, M. A., "Molecular Rectifiers," *Chem. Phys. Lett.*, Vol. 29, 1974, pp. 277-283.

[14] Aviram, A., Joachim, C., and Pomerantz, M., "Evidence of Switching and Rectification by a Single Molecule Effected with a Scanning Tunneling Microscope," *Chem. Phys. Lett.*, Vol. 146, No. 6, 1988, pp. 490-495. Errata, *Chem. Phys. Lett.*, Vol. 162, 1989, p. 416.

[15] Aviram, A., "Molecules for Memory, Logic, and Amplification," *J. Am. Chem. Soc.*, Vol. 110, 1988, pp. 5687-5692.

[16] Aviram, A., ed., "Molecular Electronics: Science and Technology," *AIP Conf. Proc. 262*, AIP Press, New York, 1992.

[17] Aviram, A., "A Strategic Plan for Molecular Electronics," *Int. J. Quantum Chem.*, Vol. 42, 1992, pp. 1615-1624.

[18] Avouris, P., "Manipulation of Matter on the Atomic and Molecular Levels," *Acc. Chem. Res.*, Vol. 28, 1995, pp. 95-102.

[19] Baggot, J., *The Meaning of Quantum Theory: A Guide for Students of Chemistry and Physics*, Second edition, Oxford U. Press, Oxford, U.K., 1992.

[20] Bain, C. D., and Whitesides, G. M., "Formation of Monolayers by the Coadsorption of Thiols on Gold: Variation in the Length of the Alkyl Chain," *J. Am. Chem. Soc.*, Vol. 111, 1989, pp. 7164-7175.

[21] Bakshi, P., Broido, D. A., and Kempa, K., "Spontaneous Polarization of Electrons in Quantum Dashes," *J. Appl. Phys.*, Vol. 70, 1991, p. 5150.

[22] Balasingam, P., and Roychowdhury, V. P., "Nanoelectronic Functional Devices," Purdue University Technical Report, TR-EE 94-24, 1994.

[23] Ballantyne, J. M., "Si Based Nanoelectronics," SRC Technical Report T95193, SRC Cooperative Research, November 1995.

[24] Bandyopadhyay, S., Das, B., and Miller, A. E., "Supercomputing with Spin-Polarized Single Electrons in a Quantum Coupled Architecture," *Nanotechnology*, Vol. 5, 1994, pp. 113-133.

[25] Bandyopadhyay, S., and Roychowdhury, V. P., "Computational Paradigms in Nanoelectronics: Quantum Coupled Single Electron Logic and Neuromorphic Networks," *Jpn. J. Appl. Phys.*, Vol. 35, 1996, pp. 3350-3362.

[26] Bass, T. A., "Gene Genie," *Wired Magazine*, August 1995, p. 114.

[27] Bate, R. T., "The Quantum-Effect Device: Tomorrow's Transistor?" *Scientific American*, March 1988, pp. 96-100.

[28] Bate, R. T., *et al.*, "An Overview of Nanoelectronics," *Texas Instruments Technical Journal*, July-August 1989, pp. 13-20.

[29] Bate, R. T., "Nanoelectronics," *Nanotechnology*, Vol. 1, 1990, pp. 1-7.

[30] Beck, J. S., *et al.*, "A New Family of Mesoporous Molecular Sieves Prepared with Liquid Crystal Templates," *J. Am. Chem. Soc.*, Vol. 114, 1992, p. 10834.

[31] Bedrossian, P., *et al.*, "Demonstration of the Tunnel-Diode Effect on an Atomic Scale," *Nature*, Vol. 342, 1989, pp. 258-260.

[32] Behrman, E. C., *et al.*, "A Quantum-Dot Neural Network," *Proceedings for the PhysComp96 Conference*, Boston, MA, November 22-24, 1996.

[33] Benioff, P., "The Computer as a Physical System: A Microscopic Quantum Mechanical Hamiltonian Model of Computers as Represented by Turing Machines," *J. Statistical Physics*, Vol. 22, 1980, pp. 563-591.

[34] Benioff, P., "Quantum Mechanical Models of Turing Machines that Dissapate No Energy," *Phys. Rev. Lett.*, Vol. 48, 1982, pp. 1581-1585.

[35] Bennett, C. H., "Logical Reversibility of Computation," *IBM Journal of Research and Development*, November 1977, pp. 525-532.

[36] Bennett, C. H., "Demons, Engines, and the Second Law," *Scientific American*, November 1987, pp. 108-116.

[37] Bennett, C. H., "Notes on the History of Reversible Computation," *IBM Journal of Research and Development*, January 1988, pp. 16-23.

[38] Bennett, C. H., "Quantum Information and Computation," *Physics Today*, October 1995, pp. 24-30.

[39] Bennett, C. H., and Landauer, R., "The Fundamental Physical Limits of Computation," *Scientific American*, July 1985, pp 48-56.

[40] Berggren, K. K., *et al.*, "Microlithography by Using Neutral Metastable Atoms and Self-Assembled Monolayers," *Science*, Vol. 269, 1 September 1995, pp. 1255-1257.

[41] Binnig, G., *et al.*, "Surface Studies by Scanning Tunneling Microscopy," *Appl. Phys. Lett.*, Vol. 40, 1982, pp. 178-81; *Phys. Rev. Lett.*, Vol. 49, 1982, pp. 57-60.

[42] Binnig, G., and Rohrer, H., "The Scanning Tunneling Microscope," *Scientific American*, August 1985, pp. 50-56.

[43] Birge, R. R., Lawrence, A. F., and Tallent, J. R., "Quantum Effects, Thermal Statistics and Reliability of Nanoscale Molecular and Semiconductor Devices," *Nanotechnology*, Vol. 2, 1991, pp. 73-87.

[44] Birge, R. R., "Protein-Based Three-Dimensional Memory," *American Scientist*, July-August 1994, pp. 348-355.

[45] Birge, R. R., ed., "Molecular and Biomolecular Electronics," *Advances in Chemistry*, Vol. 240, American Chemical Society, Washington D.C., 1994.

[46] Bissell, R. A., *et al.*, "A Chemically and Electrochemically Switchable Molecular Shuttle," *Nature*, Vol. 369, 1994, p. 133.

[47] Bouju, X., Joachim, C., and Girard, C., "Moving Gold Atoms with an Atomic-Force-Microscope Tip: A Study of Dimer and Trimer Formation on NaCl(100)," *Phys. Rev. B*, Vol. 50, No. 11, 1994, pp. 7893-7902.

[48] Boneh, D., *et al.*, "On the Computational Power of DNA," unpublished manuscript, 1995. This paper is available on the Internet World-Wide Web at the following URL: http://www.cs.princeton.edu/~dabo/papers/biocircuit.ps

[49] Brabec, C. J., *et al.*, "Growth of Carbon Nanotubes: A Molecular Dynamics Study," *Chem. Phys. Lett.*, Vol. 236, 1995, pp. 150-155.

[50] Brown, C., "The Nuances of Nanoland," *OEM Magazine*, November 1994, p. 119.

[51] Brumfield, J. C., *et al.*, "Preparation and Characterization of Laterally Heterogeneous Polymer Modified Electrodes Using in Situ Atomic Force Microscopy," *Langmuir*, Vol. 8, No. 11, 1992, p. 2810.

[52] Bryzek, J., Petersen, K., and McCulley, W., "Micromachines on the March," *IEEE Spectrum*, May 1994, pp. 20-31.

[53] Bumm, L. A., *et al.*, "Are Single Molecular Wires Conducting?" *Science*, Vol. 271, 22 March 1996, pp. 1705-1707.

[54] Cai, Z., *et al.*, "Molecular and Supermolecular Origins of Enhanced Electronic Conductivity in Template-Synthesized Polyheterocyclic Fibrils," *Supermolecular Effects Chem. Mater.*, Vol. 3, No. 5, 1992, p. 960.

[55] Campbell, S. A., *The Science and Engineering*

of Microelectronic Fabrication, Oxford U. Press, Oxford, U.K., 1996.

[56] Capasso, F., and Kiehl, R., "Resonant Tunneling Transistor with Quantum Well Base and High-Energy Injection: A New Negative Differential Resistance Device," *J. Appl. Phys.*, Vol. 58, 1985, p. 1366.

[57] Capasso, F., "Quantum Transistors and Integrated Circuits," in *Nanotechnology*, Crandall, B. C., and Lewis, J., eds., The MIT Press, Cambridge, 1992.

[58] Carter, F. L., ed., *Molecular Electronic Devices,* Marcel Dekker, Inc., New York, 1982.

[59] Carter, F. L., ed., *Molecular Electronic Devices II,* Marcel Dekker, Inc., New York, 1987.

[60] Cen, W., Lindenfeld, P., and Fehlner, T. P., "On the Interface of Metal-Metal Multiple Bond Compounds and Organometallic Clusters: Synthesis and Structure of $Mo_2\{\mu$-$[(CO)_9Co_3(\mu_3$-$CCO_2)]\}_4[(CO)_9Co_3(\mu_3$-$CCO_2H)]_2$ and Related Compounds," *J. Am. Chem. Soc.*, Vol. 114, 1992, pp. 5451-5452. In an unpublished remark at the October 1995 DARPA ULTRA Program Review, Craig Lent suggested the compounds described in this reference might have utility in the manufacture of molecular quantum dots for quantum dot cells. See references [179–185] for discussions of quantum dot cells.

[61] Cho, A., "Molecular Beam Epitaxy," *Key Papers on Applied Physics*, American Institute of Physics, Woodbury, NY, 1994.

[62] Chou, S. Y., and Wang, Y., "Single-Electron Coulomb Blockade in a Nanometer Field-Effect Transistor with a Single Barrier," *Appl. Phys. Lett.*, Vol. 61, 1992, pp. 1591-1593.

[63] Chou, S. Y., "Single-Electron and Quantum Effects in Semiconductor Nanodevices," unpublished presentation, ARPA ULTRA Program Review, Boulder, CO, 23-26 October 1995.

[64] Chou, S. Y., Krauss, P. R., and Renstrom, P. J., "Imprint Lithography with 25-Nanometer Resolution," *Science*, Vol. 272, 5 April 1996, pp. 85-87.

[65] Cirac, J. I., and Zoller, P., "Quantum Computation with Cold Trapped Ions," *Phys. Rev. Lett.*, Vol. 74, 1995, pp. 4091-4094.

[66] Claeson, T., and Likharev, K. K., "Single Electronics," *Scientific American*, June 1992, pp. 80-85.

[67] Cohen, S. N., "The Manipulation of Genes," *Scientific American*, July 1975, p. 24.

[68] Cohen, S. N., "Transposable Genetic Elements," *Scientific American*, February 1980, p. 40.

[69] Cohen, M. I., Heine, V., and Phillips, J. C., "The Quantum Mechanics of Materials," *Scientific American*, June 1982, p. 82.

[70] Comba, P., and Hambley, T. W., *Molecular Modeling*, VCH, New York, 1995.

[71] Corcoran, E., "Diminishing Dimensions," *Scientific American*, November 1990, pp. 123-131.

[72] Cory, D. G., Fahmy, A. F., and Havel, T. F., "Nuclear Magnetic Resonance Spectroscopy: An Experimentally Accessible Paradigm for Quantum Computing," *Proceedings for the PhysComp96 Conference*, Boston, MA, 22-24 November 1996.

[73] Creighton, T. E., *Proteins*, W. H. Freeman and Co., 1984, p. 84.

[74] Crommie, M. F., Lutz, C. P., and Eigler, D. M., "Confinement of Electrons to Quantum Corrals on a Metal Surface," *Science*, Vol. 262, 8 October 1993, pp. 218-220.

[75] Curtis, C. L., *et al.*, "Fabrication of Conducting Polymer Interconnects," *Science*, Vol. 262, 24 December 1993, pp. 2014-2016.

[76] Darnell, J. E., "RNA," *Scientific American*, October 1985, p. 68.

[77] Day, H. C., and Allee, D. R., "Selective Area Oxidation of Si_3N_4 with an Ambient Scanning Tunneling Microscope," *Nanotechnology*, Vol. 7, 1996, pp. 106-109.

[78] Deutsch, D., "Quantum Theory, the Church-Turing Principle and the Universal Quantum Computer," *Proc. Roy. Soc. Lond.*, Vol. A400, 1985, pp. 96-117.

[79] Devoret, M. H., Esteve, D., and Urbina, C., "Single-Electron Transfer in Metallic Nanostructures," *Nature*, Vol. 360, 1992, pp. 547-553.

[80] Derogi, M., *et al.*, "Room-Temperature Coulomb Blockade from a Self-Assembled Molecular Nanostructure," *Phys. Rev. B*, Vol. 52, No. 12, 1995, pp. 9071-9077.

[81] DiVincenzo, D. P., "Quantum Computation," *Science*, Vol. 270, 13 October 1995, pp. 255-261.

[82] Doucet, J. P., and Weber, J., *Computer-Aided Molecular Design: Theory and Applications*, Great Britain Academic Press, London, 1996.

[83] Dresselhaus, M. S., *et al.*, *Science of Fullerenes and Carbon Nanotubes,* Academic Press, New York, 1996.

[84] Drexler, K. E., "Molecular Engineering: An Approach to the Development of General Capabilities for Molecular Manipulation," *Proc. Natl. Acad. Sci.*, Vol. U.S.A. 78, 1981, pp. 5275-5278.

[85] Drexler, K. E., *Engines of Creation*, Anchor Press/ Doubleday, Garden City, New York, 1986.

[86] Drexler, K. E., "Molecular Machinery and Molecular Electronic Devices," in *Molecular Electronic Devices II*, F. L. Carter, ed., Marcel Dekker, New York, 1987.

[87] Drexler, K. E., "Rod Logic and Thermal Noise in the Mechanical Nanocomputer," in *Proc. Third Int. Symp. on Molecular Electronic Devices*, Elesevier/North-Holland, Amsterdam, 1988.

[88] Drexler, K. E., *Nanosystems: Molecular Machinery, Manufacturing, and Computation*, John Wiley and Sons, Inc., New York, 1992.

[89] Drexler, K. E., "Strategies for Molecular Systems Engineering," in *Nanotechnology* Crandall, B. C. and Lewis, J., eds., The MIT Press, Cambridge, Massachusetts, 1992, pp. 115-146.

[90] Dwyer, D. J., and Hoffmann, F. M., eds., *Surface Science of Catalysis*, ACS Symposium Series, Vol. 482, ACS, Washington DC, 1992.

[91] Eaves, L., "Looking Inside Quantum Dots," *Nature*, Vol. 357, 1992, p. 540.

[92] Eigler, D. M., Lutz, C. P., and Rudge, W. E., "An Atomic Switch Realized with the Scanning Tunneling Microscope," *Nature*, Vol. 352, 1991, pp. 600-603.

[93] Eigler, D. M., and Schweizer, E. K., "Positioning Single Atoms with a Scanning Tunneling Microscope," *Nature*, Vol. 344, 1990, pp. 524-526.

[94] Ekstrom, P., and Wineland, D., "The Isolated Electron," *Scientific American*, August 1980, p. 104.

[95] Ellenbogen, J. C., "Quantum Density Mechanics," unpublished manuscript, February 1995. Final manuscript in preparation.

[96] Enachescu, M., Hartmann, E., and Koch, F., "Writing Electronic Nanometer Structures into Porous Si Films by Scanning Tunneling Microscopy," *Appl. Phys. Lett.*, Vol. 64, 1994, pp. 2253-2255.

[97] Epstein, A. J., Miller, J. S., "Linear Chain Conductors," *Scientific American*, October 1979, pp. 52-61.

[98] Falvo, M., *et al.*, "The Nanomanipulator: A Teleoperator for Manipulating Materials at the Nanometer Scale," to be published in the *Proc. of the International Sympos. on the Sci. and Tech. of Atomically Engineered Materials*, Richmond, VA, 30 October - 4 November 1995.

[99] Felsenfeld, G., "DNA," *Scientific American*, October 1985, p. 58.

[100] Feldheim, D., *et al.*, "Modular Assembly of Surface Heterostructures from Inorganic Clusters and Polyelectrolytes," preprint, 1995.

[101] Feldheim, D., *et al.*, "Electron Transfer in Self-Assembled Inorganic Polyelectrolyte/Metal Nanoparticle Heterostructures," to appear in *J. Am. Chem. Soc.*, 1996.

[102] Ferry, D. K., *Quantum Mechanics: An Introduction for Device Physicists and Electrical Engineers,* IOP Publishing Ltd., London, 1995.

[103] Ferry, D. K., "Nano-Device Efforts Abroad and the Need for Three-Dimensional Modeling," unpublished presentation, NEMO Nanotech Seminar, McLean, VA, 7 May 1996.

[104] Feynman, R., "There's Plenty of Room at the Bottom: An Invitation to Enter a New Field of Physics." Talk at the Annual Meeting of the American Physical Society, 29 December 1959. Reprinted in *Engineering and Science*, Vol. 23, 1960, pp. 22-36.

[105] Feynman, R. P., Leighton, R. B., and Sands, M., *The Feynman Lectures on Physics*, Volume 3, Second edition, Addison-Wesley, Reading, MA, 1963. This volume of the *Feynman Lectures* discusses principles and case studies in quantum mechanics.

[106] Feynman, R., "Simulating Physics with Computers," *Int. J. of Theoretical Physics*, Vol. 21, 1982, p. 467.

[107] Feynman, R., "Quantum Mechanical Computers," *Foundations of Physics*, Vol. 16, 1986, pp. 507-531.

[108] Foster, J., "Atomic Imaging and Positioning," in *Nanotechnology*, Crandall, B. C. and Lewis, J., eds., The MIT Press, Cambridge, Massachusetts, 1992, pp. 15-36. See also references cited therein.

[109] Fountain, T., and Duff, M., "Novel Processor Arrays," unpublished presentation, ARPA ULTRA Program Review, Boulder, CO, 23-26 October 1995.

[110] Frazier, G., "An Ideology for Nanoelectronics," in *Concurrent Computations: Algorithms, Architecture, and Technology*, Plenum Press, New York, 1988.

[111] Frazier, G., "Overview of Nanoelectronics," unpublished briefing, Texas Instruments Corp., Dallas, TX, 1995. Presented at ARPA Workshop on Future Directions for Complex and Distributed Systems, Bishop's Lodge, Santa Fe, NM, 18-20 April 1995.

[112] Fredkin, E., and Toffoli, T., "Conservative Logic," *Int. J. of Theoretical Physics*, Vol. 21, 1982, pp. 219-253.

[113] Freedman, D., "Exploiting the Nanotechnology of Life," *Science*, Vol. 254, 29 November 1991, pp. 1308-1310.

[114] Frensley, W. R., "Gallium Arsenide Transistors," *Scientific American*, February 1987, pp. 80-87.

[115] Frensley, W. R., "Wigner-Function Model of a Resonant-Tunneling Semiconductor Device," *Phys. Rev. B*, Vol. 36, No. 3., pp. 1570-1580.

[116] Fulton, T. A., and Dolan, G. J., "Observation of Single-Electron Charging Effects in Small Tunnel Junctions," *Phys. Rev. Lett.*, Vol. 59, 1987, pp. 109-112.

[117] Gabriel, K., "Engineering Microscopic Machines," *Scientific American*, September 1995, pp. 118-121.

[118] Geis, M. W., and Angus, J. C., "Diamond Film Semiconductors," *Scientific American*, October 1992, pp. 84-89.

[119] Gentili, M., Giovanella, C., and Selci, S., eds., "Nanolithography: A Borderland between STM, EB, IB, and X-Ray Lithographies," *NATO ASI Series E*, Vol. 264, 1994.

[120] Ghadiri, M. R., *et al.*, "Self-Assembling Organic Nanotubes Based on a Cyclic Peptide Architecture," *Nature*, Vol. 366, 1993, pp. 324-327.

[121] Gilbert, W., and Villa-Komaroff, L., "Useful Proteins from Recombinant Bacteria," *Scientific American*, April 1980, p. 74.

[122] Gillespie, D. T., *Quantum Mechanics Primer: An Elementary Introduction to the Formal Theory of Non-Relativistic Quantum Mechanics*, International Textbook Company Limited, New York, 1973.

[123] Gleick, J., *Genius: The Life and Science of Richard Feynman*, Pantheon-Random House, New York, 1992.

[124] Gorman, C. B., Biebuyck, H. A., and Whitesides, G. M., "Fabrication of Patterned, Electrically Conducting Polypyrrole Using a Self-Assembled Monolayer: A Route to All-Organic Circuits," preprint, 1994.

[125] Goss, C. A., *et al.*, "Imaging and Modification of Au(111) Monatomic Steps with Atomic Force Microscopy," *Langmuir*, Vol. 9, No. 11, p. 2986.

[126] Grey, F., *et al.*, "Time Resolved Atomic-Scale Modification of Silicon with a Scanning Tunneling Microscope," *J. Vacuum Science Technology B*, Vol. 12, 1994, p. 1901.

[127] Haddad, G. I., "Nanotechnology Modeling Requirements for Space (and Terrestrial) Applications," unpublished briefing, NEMO Nanotech Seminar, McLean, VA, 7 May 1996.

[128] Hall, J. S., "Nanocomputers and Reversible Logic," *Nanotechnology*, Vol. 5, 1994, pp. 157-167.

[129] Hampp, M., and Ziesel, D., "Mutated Bacteriorhodopsins," *IEEE Engrg. in Medicine and Biology*, Vol. 13, No. 1, 1994, pp. 67-74. See also references cited therein. Note that this is one of eight articles in an entire issue of the cited journal devoted to the theme of molecular electronics.

[130] Hansma, P. K., *et al.*, "Scanning Tunneling Microscopy and Atomic Force Microscopy," *Science*, Vol. 242, 14 October 1988, pp. 209-216.

[131] Hasslacher, B., "Few Electron Quantum Computing Structures and Lattice Gas Computation," in *Nanostructures and Mesoscopic Systems*, Kirk, W. P., and Reed, M. A., eds., Academic Press, New York, 1992. See also references cited therein.

[132] Hassoun, M. H., *Fundamentals of Artificial Neural Networks*, The MIT Press, Cambridge, MA, 1995.

[133] Hayes, B., "The Square Root of NOT," *American Scientist*, July-August 1995, pp. 304-308.

[134] Heath, F. G., "Large-Scale Integration in Electronics," *Scientific American*, February 1970, p. 22.

[135] Heiblum, M., and Eastman, L. F., "Ballistic Electrons in Semiconductors," *Scientific American*, February 1987, pp. 103-111.

[136] Hittinger, W. C., and Sparks, M., "Microelectronics," *Scientific American*, November 1965, p. 56.

[137] Hittinger, W. C., "Metal-Oxide-Semiconductor Technology," *Scientific American*, August 1973, pp. 48-57.

[138] Holonyak Jr., N., "John Bardeen and the Point-Contact Transistor," *Physics Today*, April 1992, pp. 36-43.

[139] Hong, F. T., ed., *Molecular Electronics: Biosensors and Biocomputers*, Plenum Press, New York, 1989.

[140] Hong, F. T., "Molecular Electronics: Science and Technology for the Future," *IEEE Engrg. in Medicine and Biology*, Vol. 13, No. 1, 1994, pp. 25-32. See also references cited therein. Note that this is the overview article for an entire issue of the cited journal that contains eight articles devoted to the theme of molecular electronics.

[141] Hopwood, D. A., "The Genetic Programming of Industrial Microorganisms," *Scientific American*, September 1981, p. 90.

[142] Hopfield, J. J., Nelson, J., and Beratan, D., "A Molecular Shift Register Based on Electron Transfer," *Science*, Vol. 241, 12 August 1988, pp. 817-819.

[143] Houston, J. E., and Michalske, T. A., "The Interfacial-Force Microscope," *Nature*, Vol. 356, 1992, pp. 266-267.

[144] Howe, R. T., *et al.*, "Silicon Micromechanics: Sensors and Actuators on a Chip," *IEEE Spectrum*, July 1990, pp. 29-35.

[145] Huang, X. K., Bazan, G., and Bernstein, G. H., "New Technique for Computation and Challenges for Electron-Beam Lithography," *J. Vacuum Science Technology B*, Vol. 11, 1993, pp. 2565-2569.

[146] Huber, C. A., *et al.*, "Nanowire Array Composites," *Science*, Vol. 263, 11 February 1994, pp. 800-802.

[147] Iafrate, G. J., *et al.*, "Capacitive Nature of Atomic-Sized Structures," *Phys. Rev. B*, Vol. 52, No. 15, 1995, pp. 10737-10739.

[148] Iijima, S., "Helical Microtubules of Graphitic Carbon," *Nature*, Vol. 354, 1991, pp. 56-58.

[149] Jackman, R. J., Wilbur, J. L., and Whitesides, G. M., "Fabrication of Submicrometer Features on Curved Substrates by Microcontact Printing," *Science*, Vol. 269, 4 August 1995, pp. 664-666.

[150] Jenkins, P. P., *et al.*, "Gallium Arsenide Transistors: Realization through a Molecularly Designed Insulator," *Science*, Vol. 263, 25 March 1994, pp. 1751-1753.

[151] Joachim, C., "The Conductance of a Single Molecule?" *New J. Chem.*, Vol. 15, 1991, pp. 223-229.

[152] Joachim, C., and Gimzewski, J. K., "Analysis of Low-Voltage I(V) Characteristics of a Single C_{60} Molecule," *Europhys. Lett.*, Vol. 30, 1995, pp. 409-414.

[153] Joachim, C., and Vinuesa, J. F., "Length Dependence of the Electronic Transparence (Conductance) of a Molecular Wire," *Europhys. Lett.*, Vol. 33, 1996, pp. 635-640.

[154] Joy, B., "The Future of Computation," in *Nanotechnology: Research and Perspectives*, B.C. and Lewis, J., eds., The MIT Press, Cambridge, 1992, pp. 269-280.

[155] Jung, T. A., *et al.*, "Controlled Room-Temperature Positioning of Individual Molecules: Molecular Flexure and Motion," *Science*, Vol. 271, 12 January 1996, pp. 181-184.

[156] Kanatzidis, M., "Conductive Polymers," *Chemical and Engineering News*, 3 December 1990, pp. 36-54.

[157] Kastner, M. A., "The Single-Electron Transistor," *Review of Modern Physics*, Vol. 64, 1992, pp. 849-858.

[158] Kastner, M. A., "Artificial Atoms," *Physics Today*, January 1993, pp. 24-31.

[159] Kendall, E. J. M., *Transistors*, Pergamon Press, Great Britain, 1969. This is a reprint collection including original papers by Shockley, Brattain, and Bardeen, the inventors of the transistor.

[160] Keyes, R. W., "Power Dissipation in Information Processing," *Science*, Vol. 168, 15 May 1970, pp. 796-801.

[161] Keyes, R. W., "Physical Limits in Semiconductor Electronics," *Science*, Vol. 195, 18 March 1977, pp. 1230-1235.

[162] Keyes, R. W., "What Makes a Good Computer Device," *Science*, Vol. 230, 11 October 1985, pp. 138-144.

[163] Keyes, R. W., "Miniaturization of Electronics and its Limits," *IBM Journal of Research and Development*, January 1988, pp. 24-28.

[164] Keyes, R. W., "The Future of Solid-State Electronics," *Physics Today*, August 1992, pp. 42-48.

[165] Keyes, R. W., "The Future of the Transistor," *Scientific American*, June 1993, pp. 70-78.

[166] Keyes, R. W., and Landauer, R., "Minimal Energy Dissipation in Logic," *IBM Journal of Research and Development*, March 1970, pp. 152-157.

[167] Kim, E., and Whitesides, G. M., "The Use of Minimal Free Energy and Self-Assembly to Form Shapes," preprint, 1994.

[168] Kitching, W., Doddrell, D., and Grutzner, J. B., "Conformational Equilibria in Cyclohexyltrimethlystannane and Cyclohexyltrimethylplumbane by Low Temperature Carbon-13 NMR Spectroscopy," *J. Organomet. Chem.*, Vol. 107, No. 1, 1976, pp. C5-C10.

[169] Kolata, G., "A Vat of DNA May Become a Vast Computer of the Future," *N.Y. Times*, 11 April 1995, p. C1.

[170] Korotkov, A. N., "Wireless Single-Electron Logic Biased by Alternating Electric Field," *Appl. Phys. Lett.*, Vol. 67, 1995, pp. 2412-2414.

[171] Korotkov, A. N., Chen, R. H., and Likharev, K. K., "Possible Performance of Capacitively-Coupled Single-Electron Transistors in Digital Circuits," *J. Appl. Phys.*, Vol. 78, 1995, pp. 2520-2530.

[172] Krieger, Y. G., "Molecular Electronics: Current State

and Future Trends," *J. Structural Chem.*, Vol. 34, 1993, pp. 896-904.

[173] Kuhn, H., "Organized Monolayer Assemblies," *IEEE Engrg. in Medicine and Biology*, Vol. 13, No. 1, 1994, pp. 33-44. See also references cited therein. Note that this is one of eight articles in an entire issue of the cited journal devoted to the theme of molecular electronics.

[174] Kumar, A., Biebuyck, H. A., and Whitesides, G. M., "Patterning Self-Assembled Monolayers: Applications in Materials Science," *Langmuir*, Vol. 10, No. 5, 1994, pp. 1498-1511.

[175] Kwok, "Electromigration and Reliability in Submicron Metallization and Multilevel Interconnections," *Materials Chemistry and Physics*, Vol. 33, 1993, pp. 176-188.

[176] Landauer, R., "Irreversibility and Heat Generation in the Computing Process," *IBM Journal of Research and Development*, July 1961, pp. 183-191.

[177] Landauer, R., "Information is Physical," *Physics Today*, May 1991, pp. 23-29.

[178] Lea, A. S., *et al.*, "Manipulation of Proteins on Mica by Atomic Force Microscopy," *Langmuir*, Vol. 8, No. 1, p. 68.

[179] Lent, C.S., "Simple Quantum Models of Coulomb Effects in Semiconductor Nanostructures," in *Nanostructures and Mesoscopic Systems*, Kirk, W. P., Reed, M. A., eds., Academic Press, Inc., New York, 1992, pp. 183-193.

[180] Lent, C. S., Tougaw, P. D., and Porod, W., "Bistable Saturation in Coupled Quantum Dots for Quantum Cellular Automata," *Appl. Phys. Lett.*, Vol. 62, 1993, pp. 3558-3565.

[181] Lent, C. S., *et al.*, "Quantum Cellular Automata," *Nanotechnology*, Vol. 4, 1993, p. 49.

[182] Lent, C. S., *et al.*, "Quantum Cellular Automata: The Physics of Computing with Arrays of Quantum Dot Molecules," in *Proc. of the Workshop on Physics and Computation–PhysComp94*, 1994, pp. 5-13.

[183] Lent, C.S., lecture at the Massachusetts Institute of Technology, unpublished, February 1995.

[184] Lent, C. S., "Quantum Computation and its Perspective," report to the R&D Association for Future Electron Devices, 1995.

[185] Lent, C. S., *et al.*, "Quantum Cellular Neural Networks," extended abstract, *Proceedings for the PhysComp96 Conference*, Boston, MA, 22-24 November, 1996.

[186] Lent, C. S., private communication, June 1996.

[187] Leobandung, E., Guo, L., and Chou, S. Y., "Single Hole Quantum Dot Transistors in Silicon," *Appl. Phys. Lett.*, Vol. 67, 1995, pp. 2338-2340.

[188] Levin, C., "How Far Out is Nanotechnology," *PC Magazine*, 8 February 1994, p. 32.

[189] Lieberman, M., *et al.*, "Self-Assembly Approach to Protein Design," *Nanotechnology*, Vol. 2, 1991, pp. 203-205.

[190] Lii, J. H., and Allinger, N. L., "Molecular Mechanics. The MM3 Force Field for Hydrocarbons. 2. Vibrational Frequencies and Thermodynamics," *J. Am. Chem. Soc.*, Vol. 111, 1989, pp. 8566-8575.

[191] Lii, J. H., and Allinger, N. L., "Molecular Mechanics. The MM3 Force Field for Hydrocarbons. 3. The van der Waals' Potentials and Crystal Data for Aliphatic and Aromatic Hydrocarbons," *J. Am. Chem. Soc.*, Vol. 111, 1989, pp. 8576-8582.

[192] Likharev, K. K., "Correlated Discrete Transfer of Single Electrons in Ultrasmall Tunnel Junctions," *IBM Journal of Research and Development*, January 1988, pp. 144-158.

[193] Likharev, K. K., private communication, November 1995. The authors would like to thank Prof. Likharev for helping them to clarify certain discussions in this paper.

[194] Lindoy, Leonard F., "Marvels of Molecular Device," *Nature*, Vol. 364, 1993, pp.17-18.

[195] Lipton, R. J., "Speeding Up Computations via Molecular Biology," unpublished manuscript, 1994. This paper is available on the Internet at the following URL: ftp://ftp.cs.princeton.edu/pub/people/rjl/bio.ps

[196] Lipton, R. J., "Using DNA to Solve NP-Complete Problems," *Science*, Vol. 268, 28 April 1995, pp. 542-545.

[197] Lloyd, S., "A Potentially Realizable Quantum Computer," *Science*, Vol. 261, 17 September 1993, pp. 1569-1571.

[198] Lloyd, S., "Envisioning a Quantum Supercomputer," *Science*, Vol. 263, 4 February 1994, p. 695.

[199] Lloyd, S., "Quantum-Mechanical Computers," *Scientific American*, October 1995, pp.140-145.

[200] Luscombe, J. H., and Frensley, W. R., "Models for Nanoelectronic Devices," *Nanotechnology*, Vol. 1, 1990, pp. 131-140.

[201] Luscombe, J. H., "Current Issues in Nanoelectronic Modeling," *Nanotechonology*, Vol. 4, 1993, pp. 1-20.

[202] Lyding, J. W., *et al.*, "Nanometer Scale Patterning and Oxidation of Silicon Surfaces with an Ultrahigh Vacuum Scanning Tunneling Microscope," *J. Vacuum Science Technology B*, Vol. 6, 1994, pp. 3735-3740.

[203] Lyo, I., and Avouris, P., "Negative Differential Resistance on the Atomic Scale: Implications for Atomic Scale Devices," *Science*, Vol. 245, 22 September 1989, pp. 1369-1371.

[204] Lyo, I., and Avouris, P., "Field-Induced Nanometer to Atomic-Scale Manipulation of Silicon Surfaces with the STM," *Science*, Vol. 253, 12 July 1991, pp. 173-176.

[205] Ma, T. S., "Applications and Limitations of Polymerase Chain-Reaction Amplification," *Chest*, Vol. 108, 1995, pp. 1393-1404.

[206] Mainieri, R., private communication, 1995.

[207] Mainieri, R., "Design Constraints for Nanometer Scale Quantum Computers," preprint, 1995. Submitted to *Nanotechnology*.

[208] Marrian, C. R. K., *et. al.*, "Low Voltage Electron Beam Lithography in Self-Assembled Ultrathin Films with the Scanning Tunneling Microscope," *Appl. Phys. Lett.*, Vol. 64, 1994, pp. 390-392.

[209] Martin, A. S., Sambles, J. R., and Ashwell, G. J., "Molecular Rectifier," *Phys. Rev. Lett.*, Vol. 70, 1993, pp. 218-221.

[210] Mathias, J. P., *et al.*, "Self-Assembly through Hydrogen Bonding: Preparation of a Supramolecular Aggregate Composed of Ten Molecules," *Angew. Chem. Int. Ed. Engl.*, Vol. 32, No. 12, 1993, pp. 1766-1769.

[211] Mazor, S., "The History of the Microcomputer–Invention and Evolution," *Proceedings of the IEEE*, Vol. 83, 1995, pp. 1601-1608.

[212] McCord, M. A., and Pease, R. F. W., "Lift-Off Metallization using Poly(Methyl Methacrylate) Exposed with a Scanning Tunneling Microscope," *J. Vacuum Science Technology B*, Vol. 6, No. 1, 1987, pp. 293-296.

[213] Meindl, J. D., "Chips for Advanced Computing," *Scientific American*, October 1987, pp. 78-88.

[214] Meindl, J. D., "Limits and Opportunities for Low Power, Gigascale Integration," unpublished presentation, ARPA ULTRA Program Review, Boulder, CO, 23-26 October 1995.

[215] Meindl, J. D., and De, V. K., "A Prospectus for Gigascale Integration (GSI) Beyond 2004," SRC Technical Report T95190, SRC Cooperative Research, November 1995.

[216] Merkle, R. C., "Computational Nanotechnology," *Nanotechnology*, Vol. 2, 1991, pp. 134-141.

[217] Merkle, R. C., and Drexler, K. E., "Helical Logic," preprint, 1992. Submitted to *Nanotechnology*.

[218] Merkle, R. C., "Self Replicating Systems and Molecular Manufacturing," *J. British Interplanetary Society*, Vol. 45, 1992, pp. 407-413. This paper is available on the Internet World-Wide Web at the following URL: http://nano.xerox.com/nanotech/selfRepJBIS.html

[219] Merkle, R.C., "Molecular Manufacturing: Adding Positional Control to Chemical Synthesis," *Chemical Design Automation News*, Vol. 8, No. 9 & 10, 1993, p. 1. This paper is available on the Internet World-Wide Web at the following URL: http://nano.xerox.com/nanotech/CDAarticle.html

[220] Merkle, R. C., "Reversible Electronic Logic Using Switches," *Nanotechnology*, Vol. 4, 1993, pp. 21-40.

[221] Messiah, A., *Quantum Mechanics*, Vols. I and II, North-Holland Publishing Company-John Wiley and Sons, Inc., Amsterdam-New York, 1958.

[222] Meyerson, B. S., "High Speed Silicon Germanium Electronics," *Scientific American*, March 1994, pp. 62-67.

[223] Mikkelson, C. H., *et al.*, "Coupled-Quantum-Well Field-Effect Resonant Tunneling Transistor for Multi-Valued Logic/Memory Applications," *IEEE Transactions on Electron Devices*, Vol. 41, No. 2, 1994, pp. 132-137.

[224] Minne, S. C., *et al.*, "Fabrication of 0.1 Micrometer Metal Oxide Semiconductor Field-Effect Transistors with the Atomic Force Microscope," *Appl. Phys. Lett.*, Vol. 66, 1995, pp. 703-705.

[225] Mujica, V., Kemp, M., and Ratner, M. A., "Electron Conduction in Molecular Wires. I. A Scattering Formalism," *J. Chem. Phys.*, Vol. 101, 1994, pp. 6849-6855.

[226] Mujica, V., Kemp, M., and Ratner, M. A., "Electron Conduction in Molecular Wires. II. Application to Scanning Tunneling Microscopy," *J. Chem. Phys.*, Vol. 101, 1994, pp. 6856-6864.

[227] Mujica, V., *et al.*, "Current-Voltage Characteristics of Molecular Wires: Eigenvalue Staircase, Coulomb Blockade, and Rectification," *J. Chem. Phys.*, Vol. 104, 1996, pp. 7296-7305.

[228] Muller, R. S., and Kamins, T. I., *Device Electronics for Integrated Circuits*, John Wiley and Sons, Inc., New York, 1986.

[229] Mullis, K. B., "The Unusual Origin of the Polymerase Chain Reaction," *Scientific American*, April 1990, p. 56-65.

[230] Mullis, K. B., Ferre, F., and Gibbs, R.A., eds., *The Polymerase Chain Reaction*, Birkhäuser, Boston, 1994.

[231] Nakajima, Y. *et al.*, "Fabrication of a Silicon Quantum Wire Surrounded by Silicon Dioxide and its Transport Properties," *Appl. Phys. Lett.*, Vol. 65, 1994, pp. 2833-2835.

[232] Nespurek, S., and Sworakowski, J., "Electroactive and Photochromic Molecular Materials for Wires, Switches, and Memories," *IEEE Engrg. in Medicine and Biology*, Vol. 13, No. 1, 1994, pp. 45-57. See also references cited therein. Note that this is one of eight articles in an issue of the cited journal devoted to the theme of molecular electronics.

[233] Noge, H., Shimizu, A., and Sakaki, H., "On the Possibilities and Problems of Semiconductor Quantum Microstructures," *Nanotechnology*, Vol. 3, 1992, pp. 180-184.

[234] Noyce, R. N., "Microelectronics," *Scientific American*, September 1977, p. 62. Note that this is the overview article for an entire issue of the cited journal devoted to aspects of integrated circuit devices as they were viewed in 1977. The author of this article, Robert Noyce, is one of the inventors of the integrated circuit.

[235] Panish, M. B., "Molecular Beam Epitaxy," in *Molecular Beam Epitaxy*, Cho, A., ed., AIP Press, New York, 1994, pp. 509-518.

[236] Park Scientific Instruments, *A Practical Guide to Scanning Probe Microscopy*, Park Scientific Instruments, Sunnyvale, CA, 1996. This publication is also available on the Internet World-Wide Web at the following URL: http://www.park.com/contents.htm

[237] Parr, R. G., and Yang, W., "Density-Functional Theory of the Electronic Structure of Molecules," in *Ann. Rev. Phys. Chem.*, Vol. 46, Strauss, H. L., Babcock, G. T., and Leone, S., eds., Annual Reviews, Inc., Palo Alto, CA, 1995. This paper updates the work in reference [313].

[238] Peterson, I., "Computing with Charged Quantum-dot Arrays," *Science News*, 3 December 1994, p. 375.

[239] Pickett, W. E., Pederson, M. R., and Davidson, B. N., "Modeling CVD Diamond with Density Functional Theory," *Nanotechnology*, Vol. 5, 1994, pp. 172-178.

[240] Pierret, R. F., *Semiconductor Device Fundamentals*, Addison-Wesley Publishing Company, New York, 1996.

[241] Pool, R., "The Children of the STM," *Science*, Vol. 247, 9 February 1990, pp. 634-636.

[242] Ptashne, M., and Gilbert, W., "Genetic Repressors," *Scientific American*, June 1970, p. 36.

[243] Queisser, H., *The Conquest of the Microchip*, Harvard University Press, Cambridge, MA, 1988.

[244] Rabaey, J. M., *Digital Integrated Circuits: A Design Perspective*, Prentice Hall, NJ, 1996.

[245] Randall, J. N., "A Lateral-Resonant-Tunneling Universal Quantum-Dot Cell," *Nanotechnology*, Vol. 4, 1993, pp. 41-48.

[246] Randall, J., *et. al*, "Resonant Tunneling Devices and Logic Circuits: Lateral Tunneling Devices," unpublished briefing, Texas Instruments Corp., Dallas, TX, 1995. Presented at the ARPA ULTRA Program Review, Boulder, CO, 23-26 October 1995.

[247] Reed, M. A., Randall, J. N., and Luscombe, J. H., "Non-Equilibrium Quantum Dots: Transport," *Nanotechnology*, Vol. 1, 1990, pp. 63-66.

[248] Reed, M. A., "Quantum Dots," *Scientific American*, January 1993, pp. 118-123.

[249] Reed, M. A., "Quantum Constructions," *Science*, Vol. 262, 8 October 1993, p. 195.

[250] Reed, M. A., "Conductance Measurements of Single Atom and Molecular Systems," NATO Advanced Research Workshop, 6-10 May 1996, unpublished abstract.

[251] Reed, M. A., *et al.*, "Observation and Conductance at Room Temperature Coulomb Blockade in a Molecule," preprint, July 1996. Submitted to *Science*.

[252] Ridenour, L. N., "A Revolution in Electronics," *Scientific American*, August 1951, p. 13.

[253] Rockett, F. H., "The Transistor," *Scientific American*, September 1948, p. 52.

[254] Ross, P., "Buckytubes," *Scientific American*, December 1991, p. 24.

[255] Rousset, V., *et al.*, "Fabrication of Submicrometre Buried Gold-Palladium Wires on MoS_2 Using Electron Beam Lithography," *Nanotechnology*, Vol. 7, 1996, pp. 144-152.

[256] Roychowdhury, V. P., "Collective Computational Activity in Self-Assembled Arrays of Quantum Dots: A Novel Neuromorphic Architecture for Nanoelectronics," to appear in *IEEE Trans. Elec. Dev.*, 1996.

[257] Rubel, S., *et al.*, "Nanofabrication and Rapid Imaging with a Scanning Tunneling Microscope," *J. Vacuum Science Technology B*, Vol. 12, 1993, pp. 1894-1897.

[258] Saenz, J. J., and Garcia, N., "Quantum Atom Switch: Tunneling of Xe Atoms," *Phys. Rev. B-Condensed Matter*, Vol. 47, 1993, pp. 7537-7541.

[259] Sah, C., *Fundamentals of Solid-State Electronics*, World Scientific, Singapore, 1991.

[260] Samanta, M. P., *et al.*, "Electronic Conduction through Organic Molecules," preprint, 1995. Submitted to *Phys. Rev.*

[261] Sambles, J. R., and Martin, A. S., "Molecular Rectification," *Physica Scripta*, Vol. T49B, 1993, pp. 718-720.

[262] Schaefer, D. M., *et al.*, "Fabrication of Two-Dimensional Arrays of Nanometer-Size Clusters with the Atomic Force Microscope," *Appl. Phys. Lett.*, Vol. 66, 1995, pp. 1012-1014.

[263] Schmid, H., and Fink, H. W., "Mechanical and Electronic Manipulation of Nanometer Sized Wires," *Nanotechnology*, Vol. 5, 1994, p. 26.

[264] Schneider, H. J., Price, R., and Keller, T., "Conformational Studies by Low Temperature Carbon-13 NMR Spectroscopy," *Agnew. Chem., Int. Ed. Engl.*, Vol. 10, No. 10, 1971, pp. 730-1.

[265] Schneider, T. D., "Sequence Logos, Machine/Channel Capacity, Maxwell's Demon, and Molecular Computers: A Review of the Theory of Molecular Machines," *Nanotechnology*, Vol. 5, 1994, pp. 1-18.

[266] Scholten, R. E., *et al.*, "Nanostructure Fabrication via Direct Writing with Atoms Focused in Laser Fields," *J. Vacuum Science Technology B*, Vol. 12, 1994, p. 1847.

[267] Schumm, J. S., Pearson, D. L., and Tour, J. M., "Iterative Divergent/Convergent Approach to Linear Conjugated Oligomers by Successive Doubling of the Molecular Length: A Rapid Route to a 128Å-Long Potential Molecular Wire," *Angew. Chem. Int. Ed. Engl.*, Vol. 33, 1994, pp. 1360-1363.

[268] Seabaugh, A. C., *et al.*, "Pseudomorphic Bipolar Quantum Resonant Tunneling Transistor," *IEEE Transactions on Electron Devices*, Vol. 36, No. 10, 1989, pp. 2328-2334.

[269] Seabaugh, A. C., *et al.*, "Resonant Transmission in the Base/Collector Junction of a Bipolar Quantum-Well Resonant Tunneling Transistor," *Appl. Phys. Lett.*, Vol. 59, 1991, pp. 3413-3415.

[270] Seabaugh, A. C., Kao, Y. C., and Yuan, H. T., "Nine-State Resonant Tunneling Diode Memory," *IEEE Electron Device Letters*, Vol. 13, No. 9, 1992, pp. 479-481.

[271] Seabaugh, A. C., Luscombe, J. H., and Randall, J. N., "Quantum Functional Devices: Present Status and Future Prospects," *Future Electron Devices (FED) Journal*, Vol. 3, Suppl. 1, 1993, pp. 9-20.

[272] Seabaugh, A. C., *et al.*, "Co-Integrated Resonant Tunneling and Heterojunction Bipolar Transistor Full Adder," *IEDM*, 1993, pp. 419-422.

[273] Seeman, N. C., "The Use of Branched DNA for Nanoscale Fabrication," *Nanotechnology*, Vol. 2, 1991, pp. 149-159.

[274] Seitz, C. L., and Matisoo, J., "Engineering Limits on Computer Performance," *Physics Today*, May 1984, pp. 38-45.

[275] Semiconductor Industry Association, *The National Technology Roadmap for Semiconductors*, Sematech, Austin, TX, 1994.

[276] Service, R. F., "Mixing Nanotube Structures to Make a Tiny Switch," *Science*, Vol. 271, 1 March 1996, p. 1232.

[277] Shedd, G. M., and Russell, P. E., "The Scanning Tunneling Microscope as a Tool for Nanofabrication," *Nanotechnology*, Vol. 1, 1990, pp. 67-80.

[278] Shor, P., "Algorithms for Quantum Computations: Discrete Log and Factoring," *Proc. 35th Ann. Symp. Foundations of Computer Science*, 1994.

[279] Smith, H. I., and Schattenburg, M. L., "X-Ray Lithography from 500 to 30 nm: X-Ray Nanolithography," *IBM Journal of Research and Development*, May 1993, p. 319.

[280] Somorjai, G. A., "Surface Reconstruction and Catalysis," *Ann. Rev. Phys. Chem.*, Vol. 45, Annual Reviews, Inc., Palo Alto, CA, 1994, pp. 721-751.

[281] Somorjai, G. A., "The Surface Science of Heterogeneous Catalysis," *Surf. Sci.*, Vol. 300, 1994, pp. 849-866.

[282] Sparks, M., "The Junction Transistor," *Scientific American*, July 1952, p. 28.

[283] Stix, G., "Micron Machinations," *Scientific American*, November 1992, pp. 106-117.

[284] Stix, G., "Toward 'Point One'," *Scientific American*, February 1995, pp. 90-95.

[285] Stroscio, J., and Eigler, D. M., "Atomic and Molecular Manipulation with the Scanning Tunneling Microscope," *Science*, Vol. 254, 29 November 1991, pp. 1319-1326.

[286] Su, B., Goldman, V. J., and Cunningham, J. E., "Observation of Single-Electron Charging in Double-Barrier Heterostructures," *Science*, Vol. 255, 17 January 1992, pp. 313-315.

[287] Sundaram, M., *et al.*, "New Quantum Structures," *Science*, Vol. 254, 29 November 1991, pp. 1326-1335.

[288] Sze, S. M., ed., *High Speed Semiconductor Devices*, John Wiley and Sons, Inc., New York, 1990.

[289] Taddiken, *et al.*, "Application of Resonant Tunneling Devices in Future Electronic Circuits," in *Proc. of the Govt. Microcircuit Applications Conf.: 18th Digest of Technical Papers*, 1992, pp. 13-16. (Provided by Dr. Gary Frazier of Texas Instruments Corp., Dallas, TX.)

[290] Takahashi, Y., *et al.*, "Fabrication Techniques for Si Single-Electron Transistor Operating at Room-Temperature," *Electronics Letters*, Vol. 31, 1995, pp. 136-137.

[291] Takeda, S., Soda, G., and Chihara, H., "Solid Neopentane $C(CH_3)_4$ as Studied by Nuclear Magnetic Resonance: A Detailed Examination of Methyl and Molecular Reorientation in the Low Temperature Phase," *Mol. Phys.*, Vol. 47, No. 3, 1982, pp. 501-17.

[292] Takeuchi, S., "A Simple Quantum Computer: Physical Realization of the Deutsch-Josza Algorithm with Linear Optics" *Proceedings for the PhysComp96 Conference*, Boston, MA, November 22-24, 1996.

[293] Taniguchi, N., "On the Basic Concept of Nanotechnology," *Proc. Int. Conf. Prod. Eng.*, Tokyo, Japan, 1974, pp. 18-23.

[294] Tirrell, J. G., *et al.*, "Biomolecular Materials," *Chemical and Engineering News*, 19 December 1994, pp. 40-51.

[295] Toffoli, T., and Biafore, M., "Tailoring Cellular Automata Architectures to Arrays of Nanoscale Structures," paper, DARPA ULTRA Meeting, Santa Fe, NM, 10 October 1994.

[296] Toffoli, T., and Margolus, N., *Cellular Automata Machines*, MIT Press, Cambridge, MA, 1987.

[297] Toffoli, T., "Power Management Alternatives for Nanoscale Cellular Automata," paper, DARPA ULTRA Meeting, Santa Fe, NM, 10 October 1994.

[298] Tolles, W. M., "Nanoscience and Nanotechnology in Europe," Naval Reserach Laboratory Technical Report, 30 December 1994.

[299] Tolles, W. M., "Nanoscience and Nanotechnology in Europe," *Nanotechnology*, Vol. 7, 1996, pp. 59-105.

[300] Toth, G., *et al.*, "Quantum Cellular Neural Networks," to appear in *Superlattices and Microstructures*, 1996.

[301] Tour, J. M., Wu, R., and Schumm, J. S., "Approaches to Orthogonally Fused Conducting Polymers for Molecular Electronics," *J. Am. Chem. Soc.*, Vol. 112, 1990, pp. 5662-5663.

[302] Tour, J. M., Wu, R., and Schumm, J. S., "Extended Orthogonally Fused Conducting Oligomers for Molecular Electronic Devices," *J. Am. Chem. Soc.*, Vol. 113, 1991, pp. 7064-7066.

[303] Tour, J. M., *et. al.*, "Self-Assembled Monolayers and Multilayers of Conjugated Thiols, α,ω-Dithiols, and Thioacetyl-Containing Adsorbates. Understanding Attachments between Potential Molecular Wires and Gold Surfaces," *J. Am. Chem. Soc.*, Vol. 117, 1995, pp. 9529-9534.

[304] Tour, J. M., private communications, Spring and Summer 1996.

[305] Tucker, J. R., "Complementary Digital Logic Based on the 'Coulomb Blockade'," *J. Appl. Phys.*, Vol. 72, 1992, pp. 4399-4413.

[306] Turton, R., *The Quantum Dot: A Journey into the Future of Microelectronics*, Oxford U. Press, Oxford, U.K., 1995.

[307] Van der Wagt, P., Frazier, G., and Tang, H., "High Density Memory Based on Quantum Device Technology," in *The Proceedings of the International Conference on Integrated Micro/Nanotechnology for Space Applications*, Houston, TX, 30 October to 3 November 1995.

[308] Van der Wagt, P., Frazier, G., and Tang, H., "High Density Memory Based on Quantum Device Technology," unpublished briefing, Texas Instruments Corp., Dallas, TX, 1995. Presented at the International Conference on Integrated Micro/Nanotechnology for Space Applications, Houston, TX, 30 October to 3 November 1995.

[309] Wada, Y., *et al.*, "A Proposal of Nanoscale Devices Based on Atom/Molecule Switching," *J. Appl. Phys.*, 15 December 1993, pp. 7321-7328.

[310] Wahl, A. C., "Chemistry by Computer," *Scientific American*, April 1970, p. 54.

[311] Waldeck, D. H., and Beratan, D. N., "Molecular Electronics: Observation of Molecular Rectification," *Science*, Vol. 261, 30 July 1993, pp. 576-577.

[312] Wang, C. T., ed., *Introduction to Semiconductor Technology: GaAs and Related Compounds*, John Wiley and Sons, Inc., New York, 1990.

[313] Wang, W. P., and Parr, R. G., *Density Functional Theory of Atoms and Molecules*, Oxford U. Press, Oxford, U.K., 1988. See also references cited therein. This work is updated in reference [237].

[314] Wendel, M., *et al.*, "Nanolithography with an Atomic Force Microscope for Integrated Fabrication of Quantum Electronic Devices," *Appl. Phys. Lett.*, Vol. 65, 1994, pp. 1775-1777.

[315] Whitesides, G. M., Mathias, J. P., and Seto, C. P., "Molecular Self-Assembly and Nanochemistry: A Chemical Strategy for the Synthesis of Nanostructures," *Science*, Vol. 254, 29 November 1991, pp. 1312-1318.

[316] Whitesides, G. M., and Weisbecker, C. S., "Measurements of the Conductivity of Individual 10 nm Carbon Nanotubes," *Materials Research Soc. Symp. Proc.*, Vol. 349, 1994, pp. 263-268.

[317] Whitesides, G. M., *et al.*, "Noncovalent Synthesis: Using Physical-Organic Chemistry to Make Aggregates," *Accounts of Chemical Research*, Vol. 28, 1995, pp. 37-44.

[318] Whitesides, G. M., "Self-Assembling Materials," *Scientific American*, September 1995, pp. 146-149.

[319] Wintterlin, J., and Behm, R. J., "Adsorbate Covered Metal Surfaces and Reactions on Metal Surfaces," in *Scanning Tunneling Microscopy*, Guntherodt, H. J., and Wiesdanger, R., eds., Springer-Verlag, Berlin, 1992.

[320] Wolfram, S., "Computation Theory of Cellular Automata," *Commun. Math. Phys.*, Vol. 96, 1994, pp. 15-57.

[321] Wu, C., and Bein, T., "Conducting Polyaniline Filaments in a Mesoporous Channel Host," *Science*, Vol. 264, 17 June 1994, pp. 1757-1759.

[322] Wu, W., *et al.*, "Interface Characterization of an InP/InGaAs Resonant-Tunneling Diode by Scanning-Tunneling-Microscopy," *J. Vacuum Science Technology A*, Vol. 13, 1995, pp. 602-606.

[323] Xu, Y., Miller, S. A., and MacDonald, N. C., "Microelectromechanical Scanning Tunneling Microscope," American Physical Society March Meeting, San Jose, CA, March 20-24, 1995. *Bulletin Am. Phys. Soc.*, Vol. 40, No. 1, 1995, p. 63.

[324] Xu, Y., MacDonald, N. C., and Miller, S. A., "Integrated Micro-Scanning Tunneling Microscope," *Appl. Phys. Lett.*, Vol. 67, 1995, pp. 2305-2307.

[325] Optical computing is a fifth alternative technological approach to advanced computing. It employs coherent visible light as a basis for fast, efficient computation and dense information storage. Strictly speaking, however, visible light cannot be a basis for *nanometer-scale* computational devices. This is because the wavelengths of visible light all are longer than 100 nanometers. Thus, material structures, like waveguides, must be at least this large in optical computers. However, there have been some significant efforts to make fast, dense optical information storage/processing devices compatible with existing microelectronics and prospective nanoelectronic devices. See reference [44].

XIV. GLOSSARY

Term/Abbreviation	Definition
III/V	Alloys composed of elements from Groups III and V on the periodic table
AFM	Atomic Force Microscope
As	International symbol for element arsenic, or an arsenic atom
Au	International symbol for element gold, or a gold atom
BJT	Bipolar Junction Transistor
CPU	Central Processing Unit
DNA	Deoxyribonucleic Acid
Ga	International symbol for element gallium, or a gallium atom
GaAs	Gallium-Arsenide
GHz	GigaHertz
IC	Integrated Circuit
k	Boltzmann's constant
M	Million, i.e. 10^6
MBE	Molecular Beam Epitaxy
μm	Micrometer, one millionth of a meter, i.e., 10^{-6} meters
Micron	Abbreviated form of micrometer, one millionth of a meter
MOSFET	Metal-Oxide-Semiconductor Field Effect Transistor
nm	Nanometer, one billionth of a meter, i.e., 10^{-9} meters
N-Doped	Negatively Doped semiconductor
NEMO	Nanoelectonic Modeling program
Ni	International symbol for element nickel, or a nickel atom
NMOS	N-channel Metal-Oxide-Semiconductor. N indicates the charge of the primary carriers
NNN	Nanometer-scale Nonlinear Network
PCR	Polymerase Chain Reaction
P-Doped	Positively Doped semiconductor
QCA	Quantum Cellular Automata
Q-CNN	Quantum Cellular Neural Network
RNA	Ribonucleic Acid
RTD	Resonant Tunneling Device
SAM	Self-Assembled Monolayer
SEM	Scanning Electron Microscope
SET	Single Electron Transistor
Si	International symbol for element silicon, or a silicon atom
SRAM	Static Random Access Memory
STM	Scanning Tunneling Microscope
T	Absolute temperature in degrees Kelvin
ULSI	Ultra-Large-Scale Integrated digital circuit
UV	Ultraviolet
VLSI	Very-Large-Scale Integrated digital circuit
Xe	International symbol for element xenon, or a xenon atom