Molecular Electronics: The Experimentalist's View

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ABSTRACT

In the last few years, significant experimental advances have been achieved in the utilization of nanoscale molecular components for electronic applications. A variety of materials, including carbon nanotubes, custom-synthesized organic molecules, metallic nanoparticles, and biological molecules, have been used to build devices and simple circuits that demonstrate switching, logic and memory functions. These represent important steps in the development of molecular electronics as a possible solution to roadblocks in conventional scaling. Some of these advances are reviewed, and related topics in which complementary research in computational science can bring improved understanding or enhancements in experimental techniques are suggested.

Keywords: molecular electronics, nanotubes, synthetic molecules, DNA.

1 INTRODUCTION

As the push continues to attain ever smaller devices and increasing circuit density, the use of individual molecules as device and circuit components becomes progressively more attractive. Molecules are highly uniform in nature and inherently nanoscale in size. These two features could be very advantageous for the fabrication of ultra-dense, low-power ICs. Furthermore, organic and inorganic molecules can be synthesized with unique chemical, physical and biological properties that could be used to facilitate self-assembly to one another and to specific surfaces, and to form circuits that can perform information processing. The traditional semiconductor based approach is from the "top-down", starting with large wafers on which small components are fabricated and interconnected using lithography, metallization, etch, and other processing techniques. The "bottom-up" concept of molecular electronics represents a paradigm shift, in which the starting components are naturally nanoscale and are self-assembled into devices and circuits. This may offer significant economic advantage due to its inherent simplicity. For these reasons, research in molecular electronics has generated considerable interest in recent years.

While the concept of molecular electronics is not new and a wide variety of molecules and nanoparticles have been considered as candidates, the last few years have witnessed significant research advances. Carbon nanotubes (CNTs), with a diameter as small as 1 nm, have been fabricated into transistors and simple logic circuits [1,2]. And several custom-synthesized molecules have been shown to exhibit useful electronic functions such as switching and memory [3,4]. Meanwhile, others have used the molecular recognition properties of deoxyribonucleic acid (DNA) to facilitate the self-assembly of nanoscale structures [5]. While these molecules provide unique features, each has its own individual technical challenges as well. This, in turn, opens up many exciting opportunities in the field of computational science, some of which are described below.

2 EXPERIMENTAL ADVANCES AND OPPORTUNITIES FOR MODELLING

2.1 Carbon Nanotubes

Single wall CNTs (SWNTs) have been shown by a number of research groups to exhibit transport characteristics analogous to conventional field-effect transistors (FETs). Very recently, simple circuits including inverters, a logical NOR, a static random-access memory cell, and a ring oscillator have been demonstrated by connecting together SWNT-FETs [1,2]. This represents a significant research advance in using nanoscale components for electronic applications. However, the semiconducting behavior of these devices is still not fully understood, and the nature of the CNT-metal electrode interface remains a key factor that requires more study. Moreover, these structures are formed by the liquid phase deposition of bulk-prepared SWNTs. Quite often, the device consists of a small bundle of SWNTs instead of an individual SWNT due to the strong inter-tube interactions that results in tube bundling. The possibility of a mixture of metallic and semiconducting SWNTs in the bundle complicates the analysis. The use of selective growth by chemical vapor deposition circumvents the bundling problem. FETs with individual CNTs can be fabricated using this approach [6]. However, the development of growth methods to control the tube type (metallic or semiconducting) is still needed, and modeling advances in this area will be very beneficial.

2.2 Custom Molecules

In the last couple of years, custom-synthesized molecules have been used to demonstrate electronic functions using lithographically defined structures. An electronically addressable, bistable switch was fabricated from a single monolayer of (2)catenane sandwiched between poly-Si and Ti/Al electrodes [3]. And molecular wires of amino- and nitro-substituted phenylene ethynelenes connected to Au electrodes were shown to have electronically programmable memory [4]. This is a very fruitful area for computational research. The high flexibility in synthetic chemistry can create many combinations of molecular structures and end groups for the development of mechanisms to explain (and eventually predict) charge transport and molecule-electrode interactions. However, the challenge may be on the experimental side still since formation of the molecule-electrode interface in many cases is not well controlled as yet at the nanoscale.

Most recently, the above-mentioned 2-terminal devices have been supplemented by 3-terminal structures exhibiting FET-like characteristics [7]. These differ from previously reported organic FETs in that the channel current is carried only by a small number of molecules adjacent to the gate (i.e., not a bulk effect device). One major distinction from the 2-terminal devices is that these provide gain, and so would represent a significant improvement. Of course, a more detailed understanding of the transport mechanism needs to be developed, particularly in view of the presence of non-equivalent contacts (one self-assembled, the other evaporated) and the high current levels achieved.

2.3 DNA

Strands of DNA are highly selective in terms of molecular recognition due to the complementary nature of the base-pair sequences. This characteristic is ideally suited for self-assembly and for further integration with other nanoscale objects, leading to what might be envisioned as bio/nano devices. However, DNA is highly sensitive to temperature, pH and other environmental factors. This has a strong bearing on its chemical compatibility with other processes and molecules. One such advance in this area is the use of DNA as a template for the deposition of a 12 ?m long, 100 nm wide Ag wire, achieved by first hybridizing a DNA molecule with surface-bound oligonucleotides such that it bridged across two Au electrodes [5]. Another example is the self-assembly of nanowires into two- and three-dimensional networks. The Au regions of Au-Pt-Au segmented nanowires (35–200 nm in diameter) can be derivatized selectively relative to the Pt with single-strand DNA molecules. Then a combination of electric field- and chemical-assisted assembly techniques can be used to align and attach these segmented nanowires with good uniformity and reproducibility onto templated SiO_2 substrates [8].

In terms of using DNA as active components in electronic devices, the fundamental question as to the nature of DNA electrical conductivity is still not totally resolved. Results from earlier studies of fluorescence quenching measurements have been widely different, ranging from basically insulating properties to claims that DNA is a molecular wire [9]. More recently, however, there have been two reports of direct measurement of electrical transport through DNA molecules [10]. Linear I-V characteristics were observed at low voltages in one case, while nonlinear I-V curves with a voltage gap which increases with temperature were measured in the other. These are encouraging results but a detailed understanding of the conduction mechanism in DNA remains as a key issue in this regard.

3 SUMMARY

Significant experimental advances have been achieved in the last few years in the utilization of nanoscale molecular components for electronic applications. It is likely that research in molecular electronics will evolve in a way in which the various classes of molecules are used in combination to exploit their respective strengths. By developing techniques to customize and control properties such as charge transport, molecular recognition, and self-assembly, and by developing unique architectures that can fully utilize the benefits of nanoscale devices and circuits, a revolutionary approach to ultra-large-scale integration can be realized. Development of these methods is challenging, and will benefit significantly from insights provided by complementary research in computational science. Many opportunities for scientific and technological discovery can be expected from close collaboration between experimental and computational researchers.

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