MOLECULAR ELECTRONICS

Back under control

To some researchers, the goal of molecular electronics is to develop cheaper and higher-performance alternatives to conventional silicon-based technology. To others, it is the exploration of entirely new possibilities opened up by the different properties and phenomena exhibited by devices constructed at the molecular level. Steady progress is being made on understanding how and if these goals can be achieved.

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In the past few years, molecular electronics has been the focus of substantial research worldwide, with reports of numerous interesting devices and circuits. Significant progress has been made in the control and understanding of devices at this challenging length scale, as shown by the numerous papers presented at the March 2004 American Physical Society meeting in Montreal, Canada. In topics ranging from single-molecule transport to detailed spectroscopy of molecular devices, new fundamental understanding of these devices is beginning to emerge.

Molecular devices pose a distinct set of challenges, both in understanding and embodiment. For example, the simplest case of a molecular device would seem to be a single molecule inserted between leads, such as that shown in Fig. 1. However, this has turned out to be the most complex case, as the number of molecules, their configuration, their purity, and numerous other important variables are not known and are not amenable to known characterization tools. Even in more conventional molecular films, some of the basic questions, such as contact properties and transport mechanisms, have gone unanswered until now.

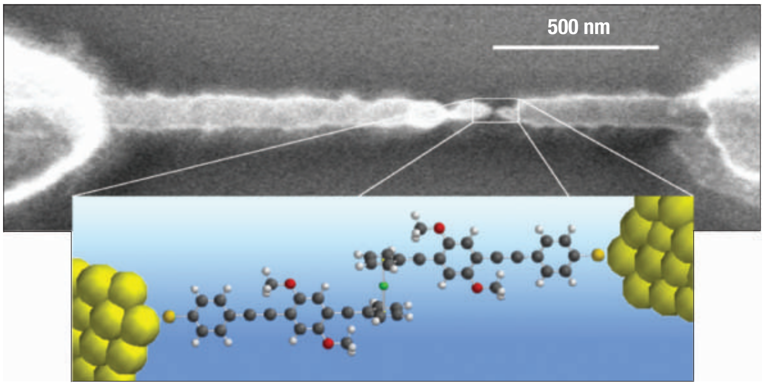

Figure 1 Scanning electron micrograph of an electromigration-fabricated gold junction, with a nanometre-scale gap, used by Stephanie Getty and co-workers at the University of Maryland, USA, to study transport through single molecules. The schematic is of the ferrocene-containing molecular wire between gold electrodes; this molecule showed a conductance of nearly 70% of the ideal quantum of conductance. Figure courtesy of Getty *et al.*

The results presented at the APS meeting were not just on applications, but a return to a more fundamental understanding with the development of standard processes, devices and controls that are sorting out intrinsic molecular transport mechanisms.

A series of experiments by Stephanie Getty and co-workers at the University of Maryland, USA, measured the electronic transport of single molecules, using a newly developed electromigrated nanoscale junction technique. Until now, single-molecule junctions have been relatively insulating because the coupling of the molecules to the metallic leads has limited the conductance. The Maryland group attempted to modify this by incorporating low redox potential organometallic centres with tailored conjugated organic linkers to the leads. When they incorporated a ferrocene centre in their conjugated molecule (Fig. 1), they obtained a conductance of nearly 70% of the ideal quantum value ($2\,e^2\,h^{-1}$, or $1/(12.9\ \mathrm{K\Omega})$), as compared with control structures with no organometallic centre, which had much lower conductance.

Numerous companion papers throughout the conference showed similar experiments on other molecules and lead configurations, demonstrating an impressive ability to tailor single-molecule junctions. One approach of particular note was given by Hugh Dalgleish and George Kirczenow from Simon Fraser University, Canada, who proposed the use of ferromagnetic contacts to form a device that they predict should act as an efficient spin-valve. Tantalizingly, preliminary experiments on similar devices performed by Sara Slater and co-workers from Cornell University, USA, may have already observed this effect.

As impressive as the single-molecule experiments have become, the precise molecular configurations of single-molecule junctions have been problematic and inaccessible to detailed structural characterization, which has limited their ability to agree with theory. The use of self-assembled monolayers has allowed devices with better-known molecular configurations to be studied, and this approach has been used by James Kushmerick at the Naval Research Laboratories, USA, and Wenyong Wang at Yale University, USA. Their results incorporate detailed structural, electrical and spectroscopic studies of molecular junctions that display an impressive agreement with theory, and provide the first detailed 'picture' of the molecules within a molecular device structure. In the NRL study, both molecules and endgroups were systematically varied to investigate their dependencies on conductivity, and the Yale group unambiguously demonstrated (through kinetic studies) the expected transport mechanisms in their specific molecular species. In addition, both groups demonstrated inelastic electron tunnelling spectroscopy of their molecular devices, a technique that can uniquely identify the presence of the molecular species (and the absence of impurities) in the junctions, yielding the first picture of the molecule in the device. These studies should provide important tools for exploring and hopefully tailoring the basic transport mechanisms of molecular devices.

An example of such novel molecular device behaviour was shown by Bonnie Ludwig and co-workers from the University of Michigan, USA, who reported a device incorporating hydridosilsesquioxane that exhibited negative differential resistance (NDR) behaviour (in which the conductivity of a device, in selected regions of device bias, decreases with increasing bias). Using an isotope substitution, they found that hydrogen plays a key role in the NDR mechanism, and suggest that it could serve more generally to mediate the formation of the current-conducting paths that give rise to this behaviour in a wide range of other metal-insulator-metal NDR devices.

With the tremendous advances made in diagnostic spectroscopies and control of molecular device fabrication, such interesting suggested mechanisms can not only be verified, but optimized. Armed with these tools, researchers should be able to reach the regime that has so far eluded them: the rational design of molecules to exhibit predicted device behaviour. The March APS meeting demonstrated tremendous progress toward a fundamental understanding of these structures.

MATERIAL WITNESS

Heavy computing

My computer has a mass of about 1.7 tonnes. So does yours. It probably doesn't feel that way, but that's the mass of the materials that went into its making.

You'll probably not be surprised to learn that most of it is water: 1.5 tonnes for a typical desktop PC with a 17-inch monitor. Most of the rest is 'embodied energy': producing this equipment requires around 240 kg of fossil fuel.

These are the figures cited by Eric Williams of the United Nations University, Japan, in *Computers and the Environment: Understanding and Managing their Impacts* (Kluwer Academic & UNU, 2003). The question is: should we worry? It's again no surprise that the manufacture of high-tech electronic devices is energy-intensive, or that the economy in materials that apparently stems from miniaturization masks a vast investment in raw materials and energy needed to build at ever-smaller scales. Thermodynamics alone tells us that we do not get such intricate organization of matter for free.

But the question is of course too simply stated. High-value-added, lightweight materials may be costly in all respects to manufacture, but they might then significantly reduce the fuel consumption of a vehicle. And what about the relative environmental impacts (and the associated costs) of different materials during manufacture or after disposal?

What's more, technical advances do seem capable of reducing the total costs of technologies: a study from 1993, based on data from the late 1980s, estimated the embodied fossil-fuel energy in a computer workstation at around 740 kg, three times the figure calculated by Williams. Improvements in processing efficiency over the past decade may account for the difference.

Perhaps the value of such studies lies primarily in forcing us to think more carefully about how we use these devices, as well as where to focus efforts to reduce their overall cost to the environment. Making a car requires around two tonnes of fossil fuels: eight times more than a computer, but nearly an order of magnitude less on a weight-to-weight basis. Perhaps even more pertinently, the typical active lifespan of a computer is a fraction of a car's. We change our car about once every ten years, but might buy a new computer every two years (and who wants the old one?).

Then there is the question of energy use over a lifespan. For a refrigerator, 96 percent of the fossil fuel consumed in its life cycle is burnt up during use; for a computer, three quarters of the total energy goes into making it, and only a quarter into powering it.

The answer, then, seems obvious: computers, or at least their parts, should be reused whenever possible. Their components, particularly the microchips (94 kg of embodied fossil fuel in each computer), represent an enormous energy investment. But somehow the economics have gone awry. Why go to the expense and trouble of upgrading your tawdry old model, which doesn't have the compatibility you need anyway? The first obsolescence-proof computer will spark a revolution.

PHILIP BALL