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A Scanning Tunneling Microscope as a Switch in a Nanocomputer

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There are several "molecular machines" that have been devised on a nanometer scale, made from proteins, DNA, and other molecules. A molecular machine is a system that generates physical forces at the atomic level, controlled by an external stimulus. Since all of the proposed circuits connect components linearly, they only communicate with one machine at a time. Now, Anirban Bandyopadhyay and Somobrata Acharya have devised an ingenious device that has the potential to communicate different instructions to many molecular machines simultaneously.² They demonstrated that 2,3,5,6-tetramethyl-1–4-benzoquinone (duroquinone; DRQ) can be assembled as 17 identical molecules, one central molecule surrounded radially by 16 others. The central molecule can control the conformation of all the others when switched to one of four logic states by suitable pulses from an atomic sharp needle of a scanning tunneling microscope (STM).

The beauty of the system is that the central DRQ molecule can execute 16 instructions at a time, and each of the 16 molecules it signals is a logic machine that can generate up to four instructions by rotating its alkyl groups. Therefore instructions executed by a STM tip on the central molecule can change decisions in four billion (4^{16}) ways!

This began with Bandyopadhyay, Acharya, and other colleagues creating a multilevel switch in DRQ that generates four logic states (0, 1, 2, and 3) within a space of 7Å when stimulated by an appropriate STM pulse. Each logic state is associated with a certain rotation of alkyl groups, so this switch fits the definition of a molecular machine. This DRQ, now referred to as the central control unit (CCU), can in turn be placed in the center of a ring of 16 other DRQ molecules which then operate as execution units (EUs). Hydrogen-bond channels originating from the central DRQ

connect radially to the 16 EUs, providing a synchronized "one-to-many" control of their logic states. This is accomplished by influencing an outer oxygen atom of a EU molecule such that it changes its negative charge by a finite amount.

Using certain properties of this arrangement of 17 DRQ molecules, particular instructions can be selectively inserted by applying a single STM pulse to the CCU. For example, an array can be changed by switching the logic state of the CCU that in turn can generate 16 instructions to the EUs, instructing some to function independently and fixing others to a specific state. In principle, all 16 bits, comprising 4¹⁶ decision sets, could be changed by a signal from the CCU.

To demonstrate a proof of concept, Bandyopadhyay and Acharya arranged to conduct 19 simultaneous operations of 8 recently-invented nanomachines (elevator, rotary fan, nano-toy, switch, bearing, flier, dual flipper, and link breaker). Each of these machines has different operational mechanisms and perform certain tasks assigned to them. Although a much larger number of machines could in theory be simultaneously controlled, certain physical limitations, such as steric hinderance, probably won't allow the full potential of this parallel processing to be realized in this architecture. However, using this concept, chemists can design systems where more (~ 1000) molecular machines could be attached and operated in parallel. Current work involving other colleagues promises to realize the potential of such systems.

It is clear that the way has been shown to control many machines on the molecular scale. The concept of simultaneous one-to-many communication could be generalized to build massive supramolecular computer architectures wherein parallel processing could be established. The potential for miniaturized yet powerful computers could be phenomenal!

- 1 The author gratefully acknowledges Dr. Anirban Bandyopadhyay for reviewing this article. He specifically wishes to acknowledge his colleagues Drs. Wakayama, Miki, Hill, and Fujita.
- 2 Bandyopadhyay, A., and S. Acharya, A 16-bit parallel processing in a molecular assembly, Proc. Nat. Acad. Sci. 105:3668-3672, 2008.

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