

fan-out (the ability of a given device to provide sufficient power to operate multiple devices interconnected to it) to reduce the wiring complexity between the gates and to lower the power dissipation per gate. The extreme fabrication constraints, especially for complex circuits, will require new architecture paradigms. For instance, it has been proposed to replace process precision by software precision⁷⁰, by using an external nonmolecular processor to select the working HME devices from a massive array of HME devices connected in a checkerboard pattern and to configure a particular circuit. In such cases gain might be localized elsewhere, using traditional CMOS (complementary metal oxide semiconductors) outside the molecular electronic circuitry, with some trade-off in space. Other architectures that have been proposed are quantum cellular automata^{55,71} and quantum computing using a molecule as a quantum dot⁷².

Mono-molecular integration

An ultimate limit of downscaling a circuit made of metallic wires interconnecting HME devices is a circuit where the wires and devices are no longer distinguishable as localized discrete elements of the circuit. This occurs when the interdevice wire length is well below the electronic phase coherence length of the wire material, so that the circuit operates in a ballistic regime where a minute difference between device positioning or wire length will render the circuit unreliable⁷³. Another limit, also experienced in integrated photonics⁷⁴ and mesoscopic low-temperature devices⁷⁵, is that true intrinsic three-terminal devices with external grids are difficult to design in a ballistic regime. A similar problem arises when a metallic control electrode is used to gate a single HME device (Fig. 2). Therefore, the scaling ability of the HME approach is limited even if SWCNTs are used to replace the metallic nanowires for interdevice wiring. Semiconductor-based electronics, when faced at the end of the 1950s with similar limitations that were based on different physical constraints, turned to monolithic technology, which integrates the wiring, transistors and the required passive elements on a single piece of silicon. The conceptually comparable mono-molecular approach (MME) was suggested for molecular electronics as early as the 1980s⁵⁵, but has only recently received serious

theoretical⁴⁰ and experimental consideration^{45,76}. Tunnelling is one way to overcome the limitations associated with the ballistic transport regime. In this case, electrons are channelled from one reservoir to the other via a network of tunnelling pathways defined by atomic or molecular wires.

The tunnel transparency T between two metallic electrodes is known to exhibit a sharp exponential decay, $T = T_0 e^{-\gamma L}$ with length L through a vacuum gap and $\gamma \approx 2 \text{ \AA}^{-1}$ (ref. 77). Low-gap semiconductor⁷⁸ or molecular materials⁹ tend to reduce the inverse decay length γ . It has been shown theoretically⁷⁹ that tunnelling currents as high as 10 pA under a 0.1-V bias voltage can be driven through specifically designed molecular wires having lengths exceeding 10 nm and a HOMO-LUMO gap in the 1-eV range. Recently, a value of $\gamma = 0.4 \text{ \AA}^{-1}$ was reported for the molecular wire 16 (Fig. 1a), equipped with supporting molecular groups (legs) that exhibit very low T that protect the conjugated wire from a Cu(100) surface. One end of the molecular wire was interconnected to a double atomic step edge and a STM tip used to explore the length dependence of its transparency⁷⁶, confirming that tunnelling electrons can be guided by long molecular wires with an effective section well below 1 nm^2 . On the electronic transport regime map (Fig. 3), this 'super tunnel'-like phenomenon corresponds to a wire with a section smaller than the de Broglie wavelength of the electron. It can be interpreted as a permanently driven super-exchange electron-transfer mechanism. Although large-scale theoretical and chemical synthesis efforts are required to model and explore this regime, theoretical considerations indicate that values of γ down to 0.05 \AA^{-1} are achievable for a HOMO-LUMO gap in the 1-eV range⁷⁹. Currently, the chemical synthesis strategies for molecular wires continue to place an emphasis on the length (Fig. 4), such as in 15 (Fig. 1a), rather than on the optimization of their γ values.

Many calculations have explored the possibility of optimizing the electronic contacts between the end of a molecular wire and a metallic electrode, as has been realized in the case of molecule 16 (ref. 76), by investigating the influence of the wire's end group^{33,36,37}. The metal-molecule contact results from a mixing of the end part of the wire's molecular orbitals (HOMO, LUMO and the others

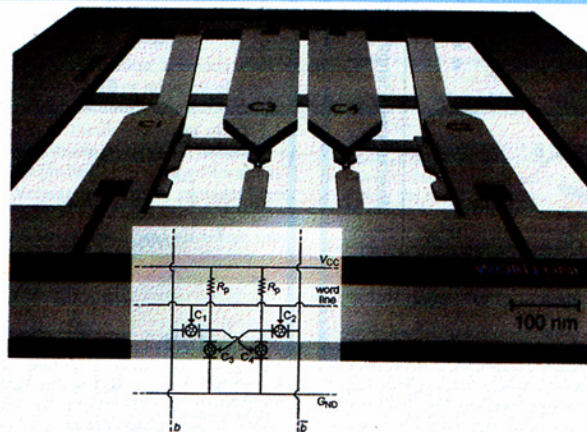


Figure 4 Representative example design of a hybrid molecular electronic device. The figure shows the layout of a memory cell that consists of four individual C_{60} electromechanical transistors⁶⁴ (two for the trigger and two for the driving transistors) under a bias voltage V_{CC} with respect to ground, G_{ND} . The top part is made of four nanoelectromechanics (NEMS) grids plus two metallic NEMS cantilevers, and the lower part is the electrical polarization circuit with polarization resistances R_p made using a metallic constriction along the mesoscopic metallic wires of the circuit (see inset). The full circuit was simulated and optimized using an equivalent electrical circuit for each cantilever and for each C_{60} molecule using the known C_{60} experimental electrical characteristics upon compression¹⁵. Inset, the equivalent electrical circuit diagram. b and \bar{b} carry the digital information to be stored in a memory cell, and the word line activates a line of memory cells for a storage operation.