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# Assembling a molecular computer: challenges in integrating molecular logic, memory, and interconnects from the "bottom-up"

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The advancement of high-performance computing is unlocking the potential of artificial intelligence and machine learning, providing significant benefits to everyday life. Miniaturization of silicon-based transistors is enabling this transformation; however, challenges such as quantum tunneling, contact resistance, and excess power consumption are significant obstacles as we approach the 5 nm limit. Molecular electronics, which replicates the function of electronic components with single molecules, offers an attractive alternative, with the molecular-scale representing the final frontier in miniaturization. Recent progress in molecular logic gates, memory units, and interconnects underscores the potential of molecular electronics to mitigate the excessive power consumption and heat generation associated with current technology. While significant progress has been made, the integration of separate components into functional devices remains limited. This review outlines the challenges of assembling molecular components within a von Neumann architecture. We discuss current challenges, highlighting successful molecular electronic case studies, and then conclude with five milestones to be reached on the journey towards the world's first functional molecular computer.

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## Introduction

Continual advances in computational technology are fuelling artificial intelligence (AI) and machine learning (ML), which are benefitting society.[1,2] The miniaturization of silicon-based transistors is enabling this transformation with state-of-the-art integrated circuits (ICs) containing billions of transistors approaching 5 nm.[3] This trend has historically followed Moore's first law: the number of transistors on a IC doubles approximately every two years.[4] Sustaining this progress required increasingly sophisticated fabrication technologies, with the construction of leading-edge fabrication facilities now exceeding $25 billion.[5] Alongside the financial cost of silicon transistor miniaturization, fundamental scientific limitations are becoming apparent. Phenomena such as quantum tunnelling,[6] high contact resistance,[7] excessive power consumption,[8] and heat dissipation[9] present formidable challenges. IC demand often outstrips supply with approx. 75% of global manufacturing centred in Asia.[10] This production bottleneck is intensifying political tensions as nations compete for these critical resources. The recent CHIPS Act in the United States of America and the European Chips Act are leading examples.[11,12] We are approaching a computing crossroad requiring research into alternative computing paradigms (Fig. 1A). Quantum computing, which leverages qubits (quantum bits) for computation, has promise in cryptography[13] and niche applications, yet its complex instrumentation and cryogenic operating temperatures limit widespread use.

Photonic computing, which utilizes light for computation, is providing advances to datacentres,[14] however, the storage of data as photons is limited, and complex fabrication limits mass production.[15] Miniaturization of electronic components underpinned previous advances (Fig. 1B) with molecular electronics, in which individual molecules replicate the function of electronic components, a promising third alternative.[16] First explored in the 1970s, molecular electronics has experienced a resurgence over the past five years (Fig. 1C), with major progress in molecular logic gates, memory elements, and interconnects.[17] This "bottom-up" approach was first envisioned by Richard Feynman in his seminal 1959 lecture "There's plenty of room at the bottom."[18] The assembly of functional molecular electronic devices is now possible with several recent case studies highlighted within. While numerous reviews[19] have discussed individual molecular components, this review specifically outlines challenges on the road towards developing the world's first molecular computer. We discuss the current von Neumann architecture underpinning current computers[20] and discuss how molecular electronics can replicate and improve upon this design. We highlight recent molecular electronic commercial

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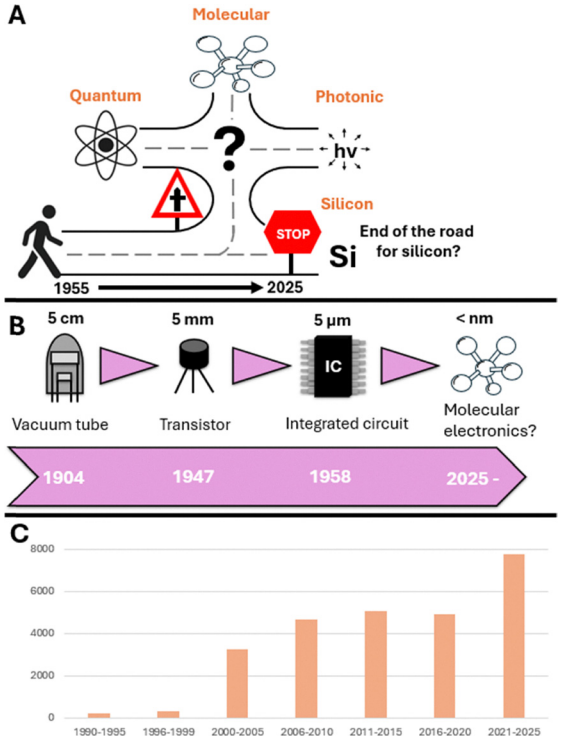



Fig. 1 The approaching computing crossroad (panel A), electronic component miniaturisation (panel B), and the rise in molecular electronics reported in the literature (panel C).

successes to demonstrate that progress is achievable. We conclude with five key milestones on the road towards constructing a fully functional molecular computer.

## The von Neumann architecture

John von Neumann (1903–1957) transformed a variety of scientific fields, including the development of ENIAC (electronic numerical integrator and computer), the world's first general-purpose computer.[20] John von Neumann would later outline a blueprint for modern computers referred to as the von Neumann architecture (Fig. 2A).[21]

This design involved a control unit that can fetch program instructions from a separate memory component, perform logic operations, and then store the resulting data in a separate part of the memory. A critical feature of this design is the programmability of the memory unit, which allows the installation of new programs or modifications to existing ones, enabling true general-purpose computing. A variety of INPUT/OUTPUT devices issue commands and observe results, while a central control unit coordinates operations and data transfers *via* a network of interconnects. Although this architecture has served as the backbone of computing for more than 70 years, the most advanced ICs reveal major limitations with this approach. First, the control unit executes tasks sequentially: it must fetch instructions from memory before performing the next operation, such as a logical computation. This sequential process has become a significant bottleneck, with even the most advanced ICs frequently left idle while waiting for instructions and data transfers. This limitation is known as the von Neumann bottleneck.[22] Second, the transfer of data from memory occurs more slowly than the ICs execution speed, referred to as the memory wall.[23] This leads to wasted energy and excess heat generation. Future computing paradigms must avoid such pitfalls. Neuromorphic computing, which mimics brain-like functions by performing operations in parallel, is a leading example.[24] For multiple molecular components to function as a cohesive unit, the five challenges (5Cs) in molecular computing must be considered.[25]

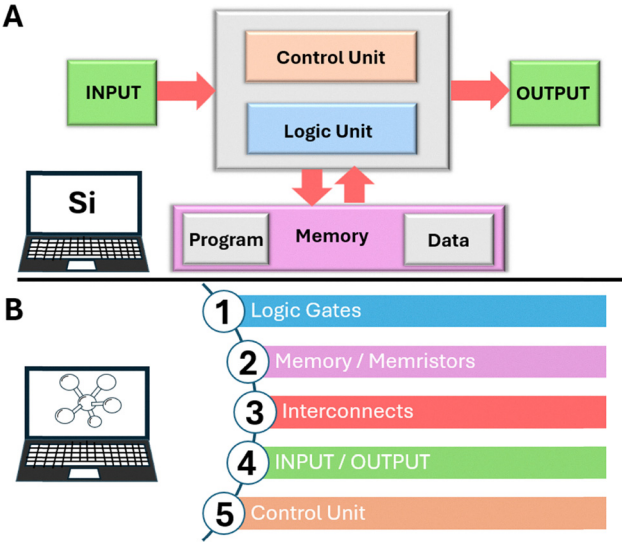



Fig. 2 The von Neumann architecture upon which all modern computers operate (panel A) and the five functions to be replicated with molecular electronics (panel B).

## The five challenges (5Cs) in molecular computing

For molecular electronics to become a practical alternative to conventional electron-based electronics, five key challenges collectively known as the 5Cs must be addressed (Fig. 3).[25] To replicate the function of silicon-based components, multiple molecular units must operate together as a coordinated system. The connection of these units, known as concatenation, is essential. To pass this challenge, the ability of two or more logic gates functioning together must be clearly demonstrated. The second challenge, connectivity, concerns the transition

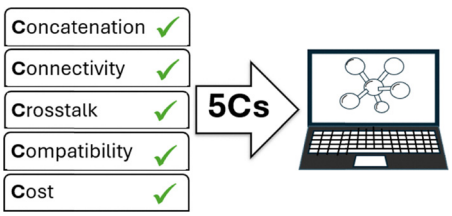



Fig. 3 The five challenges (5Cs) in molecular computing.

from solution-phase operation to substrate-bound architectures, enabling complex device fabrication. The chemical attachment of logic gates to at least one surface must be confirmed to meet this objective. Crosstalk refers to unintended signal interference with neighbouring units, which must be minimised. To achieve this challenge, the reported system must operate with clear ON/OFF signals, demonstrating robust, and repeatable operation.

Compatibility emphasizes the need for integration with existing electronic technologies. A hybrid era is highly likely, where molecular electronics coexists with conventional approaches—much as photonic integrated circuits (PICs) are already augmenting data centres today.[26] To satisfy this challenge, the reported system must be integrated with existing electronics. The final challenge is cost-effective manufacturing to ensure widespread adoption of the new technology. The use of efficient syntheses using inexpensive reagents and substrates, for example widely available industrial feedstocks, would meet this challenge. Future molecular electronics should be designed to be 5C compliant, and we will evaluate current approaches against these metrics.

## Molecular logic gates

The central feature of any computer is the ability to perform complex operations *via* the logic unit. This often takes the form of logic gates, of which there are several basic gate designs (Fig. 4).[27] These can be combined and assembled into a multitude of configurations to perform the desired tasks, for example, arithmetic. The algebraic logic underpinning these gates was first devised by George Boole in 1847, with each gate described *via* a truth table.[17c] The first molecular logic gate reported by de Silva *et al.* in 1993 was an AND gate (**1** in Fig. 4).[28] Anthracene-based **1** only triggered an output if both INPUT 1 ($H^+$) and 2 ($Na^+$) are present. The OUTPUT is fluorescence emission ($\lambda_{em}$) at a wavelength of 475 nm. This is an example of a metal-triggered INPUT producing a fluorescence OUTPUT logic gate. The opposite of an AND gate is a NAND (not AND) gate in which any combination of INPUT except both 1 and 2 INPUT together triggers an OUTPUT. Gunnlaugsson *et al.* reported the first NAND gate in 2000 with $Ca^{2+}$ and $Mg^{2+}$ as INPUT 1 and 2, respectively (**2** in Fig. 4).[29] Numerous other logic gates (**3–6**, Fig. 4) have been reported, with the majority triggering a fluorescent OUTPUT in the presence of metal INPUT. These examples confirm that molecules can replicate logic gates. In traditional silicon-based logic gates, electrons are both INPUT and OUTPUT allowing the OUTPUT of one logic gate to serve as the INPUT of another, and so on. This facilitates the connection (concatenation) of multiple logic gates. For molecular logic gates to replicate this function, we require homogeneous INPUT and OUTPUT, with light a leading contender. An excellent example, **7**, was reported by Andréasson *et al.* in 2011 based on two photochromes, dithienylethene and fulgimide (red and black units, respectively in Fig. 5).[30] Up to 14 different logic gates were reported, performing arithmetic,

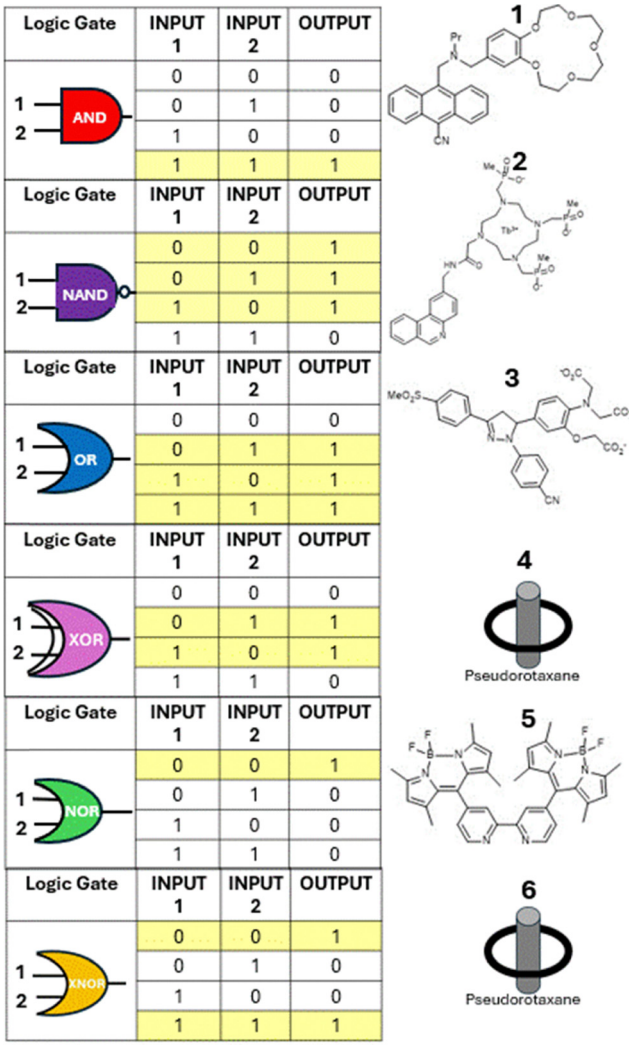



Fig. 4 The basic logic gates with corresponding truth table and molecular examples **1–6**.

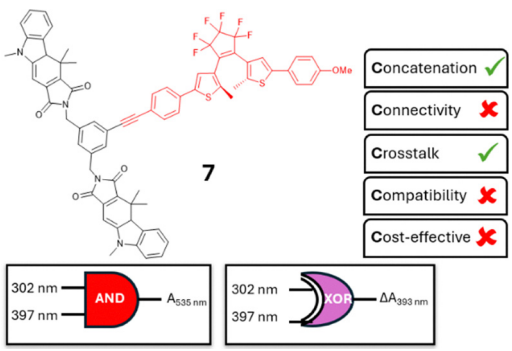



Fig. 5 The first fully photonic molecular logic gate **7** displaying multiple functions including arithmetic and keypad lock.[30]

multiplexing, and functioning as a molecular keypad lock. This system demonstrates concatenation as the OUTPUT from one logic gate serves as the INPUT for another, for example, a half-adder is composed of AND and XOR logic gates. This is a

significant result demonstrating gate-to-gate communication without any physical connection highlighting the advantages fully photonic systems provide. Furthermore, the system can be reset using an optical signal, allowing the user to undo the previous operation and reconfigure the system for a different logical operation.

Molecular logic gate **7** was solution-based, and no substrate-bound activities were reported. The photonic INPUT was also delivered by external UV sources. A further fully photonic example based on dithienylethene (red in Fig. 6) photochrome was reported in 2013 from the Andréasson and Pischel groups (molecule **8**, Fig. 6).[31] Electronics often use parity generators and checkers to ensure data transmission is free of errors. Molecule **8** can replicate this function. Dithienylethene **8** acts as a single XOR 2-bit parity generator, with the concatenation of two XOR gates serving as the parity checker. Molecule **8** was the first example of such molecular emulation of electronic parity functionality. Molecule **8** achieves the concatenation objective, however this system was solution-bound with no solid-state activities reported. A third example of dithienylethene displaying molecular logic functions was reported in 2016.[32] Molecule **9** displayed AND, OR, and INHIBIT logic gate functions, further confirming the usefulness of the dithienylethene photochrome for fully photonic molecular logic gates (Fig. 7).[32] To date, one disadvantage of this scaffold is the lack of substrate-bound reports. Substrate connectivity is essential as individual molecular components (logic gates and memory units) must function as one cohesive unit. An alternative molecular structure is spiropyran (blue unit in Fig. 8).

Spiropyran-based molecule **10** (Fig. 8) displayed fully photonic operation with AND and XOR functionality.[33] Molecule **10** serves as a half-adder *via* concatenation, enabling two binary digits to be added together. This system could be used multiple times and is a promising alternative to dithienylethene-based logic gates. In 2006 Zhu *et al.* reported spiropyran **11** bound to a gold electrode which displayed AND logic gate functionality (Fig. 9).[34] In the presence of $\lambda_{ex}$ 365 nm and $Zn^{2+}$, a change in voltage was observed. While this system is one of the first substrate-bound spiropyran molecular logic gates, the use of voltage as an OUTPUT limits the ability to concatenate multiple units together. Furthermore, the use of external UV light and

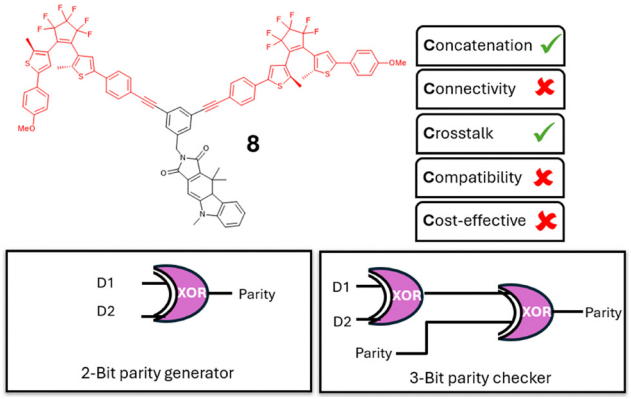



Fig. 6 A 2-bit parity generator and 3-bit parity checker.[31]

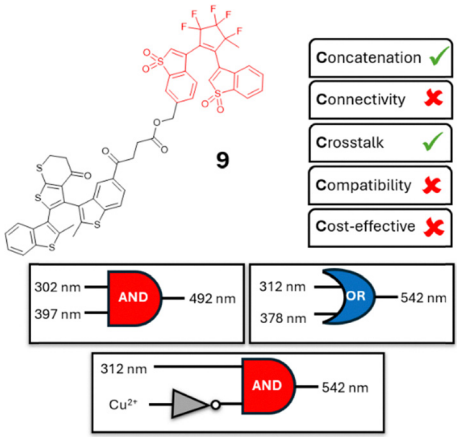



Fig. 7 Dithienylethene **9** as AND, OR and INHIBIT logic functions.[32]

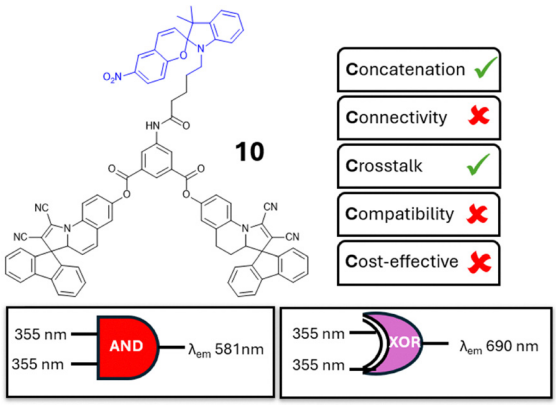



Fig. 8 Molecular logic gate **10** as a fully photonic AND and XOR gate functions.[33]

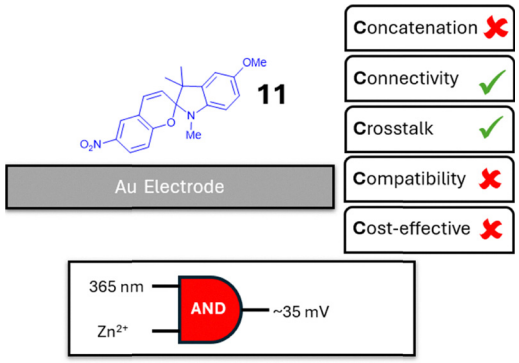



Fig. 9 Molecular logic gate **11** bound to a gold electrode.[34]

$Zn^{2+}$ as INPUTs alongside gold as the substrate limits compatibility with existing electronics and cost-effectiveness. A further spiropyran-based system, **12**, was reported by Huang *et al.* in 2007, achieving three of the five 5C criteria (Fig. 10).[35] Molecule **12** was attached to a $TiO_2$ electrode, ensuring connectivity to solid support. $TiO_2$ is a more cost-effective substrate compared to gold. This system demonstrated excellent thermal stability at

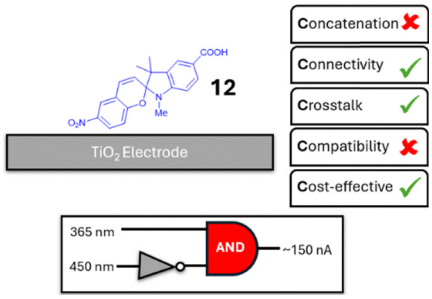



Fig. 10 Molecular logic gate **12**.[35]

room temperature however, the OUTPUT was a change in current, which limits the ability to concatenate multiple units together.

In 2014, Ming *et al.*, reported microtube-bound spiropyran **13**, which met four of the five 5C criteria (Fig. 11).[36] System **13** consists of a polydiacetylene microtube with spiropyran **13** bound to the exterior surface. The addition of **13** did not influence the waveguiding properties of the microtubes, and OR and AND logic operations could be performed. This is an excellent example of the convergence of nanomaterials and molecular electronics to solve a specific problem. The use of nanomaterials as interconnects will be discussed further. A third potential fully photonic scaffold is dihydropyrene. For example, Bandyopadhyay *et al.* reported molecule **14** bound to a range of polymers displaying fully photonic logic functionality (Fig. 12).[37]

This system complies with four of the five 5Cs and is an excellent example of solid-state application of molecular logic gates. Further applications in data storage, anti-counterfeiting, and encryption were explored. Bandyopadhyay *et al.* recently reported a fully photonic dimethyldihydropyrene solid-state dyad with logical functionality.[38] A further dihydropyrene-based molecular logic is **15** covalently attached to a porphyrin system (Fig. 13).[39] System **15** displayed AND and INHIBIT logic gate functions with photonic INPUT and OUTPUT. While no solid-state activities were reported, this example confirms compliance with three of the five 5Cs, validating the potential of dihydropyrene for future applications. Azobenzenes are another explored scaffold for the development of molecular logic gates.[40] Wang *et al.* reported azobenzene **16**, which displayed INHIBIT logic functionality and azobenzene **17** with OR functionality (Fig. 14).[41] Interestingly, both compounds displayed different mechanisms despite similar structural

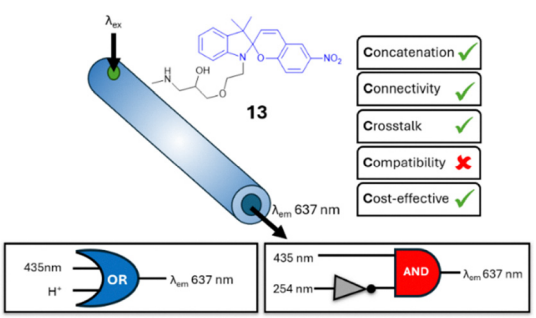



Fig. 11 Molecular logic gate **13** attached to polydiacetylene microtubes.[36]

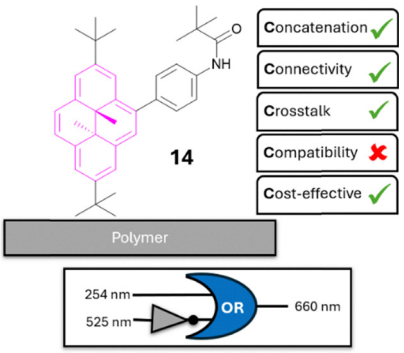



Fig. 12 Molecular logic gate **14** attached to a polymer.[37]

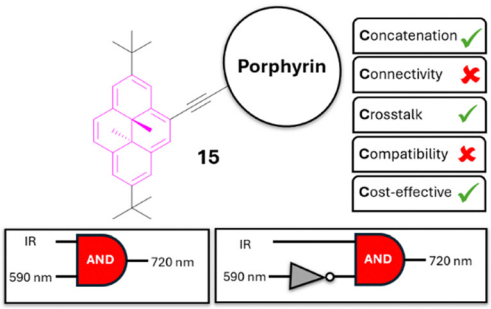



Fig. 13 Molecular logic gate **15** covalently linked to porphyrin.[39]

features. This demonstrated that the simple azobenzene unit can be easily modified for specific functionality. All studies were performed in the liquid state, and no solid-state applications were reported. The use of $OH^-$ and $Zn^{2+}$ as input limits the ability to concatenate multiple units together; therefore, this system only meets two of the five Cs.

Khanmohammadi *et al.* reported a further azobenzene molecular system which displayed both AND and OR using anions as INPUT (Fig. 14).[42] A particularly useful feature of azobenzene **18** is the concatenation of the AND and OR gates to form a "Write–Read–Erase–Read" memory unit. When the system has no Set or Reset signal (designated as $F^-$ and $Ca^{2+}$ respectively) there is no data stored in the system (entry 1 in truth table, Fig. 15). In the presence of Set INPUT ($F^-$) the system stores data and the OUTPUT is 1 (entry 2 in truth table,

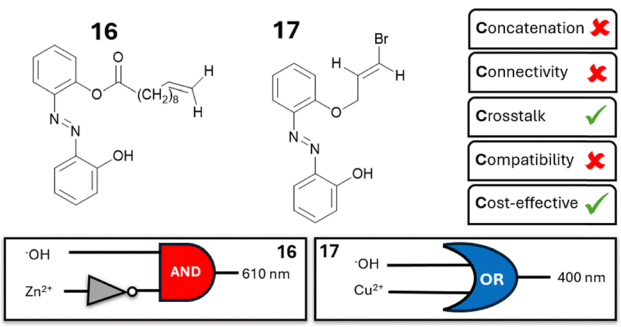
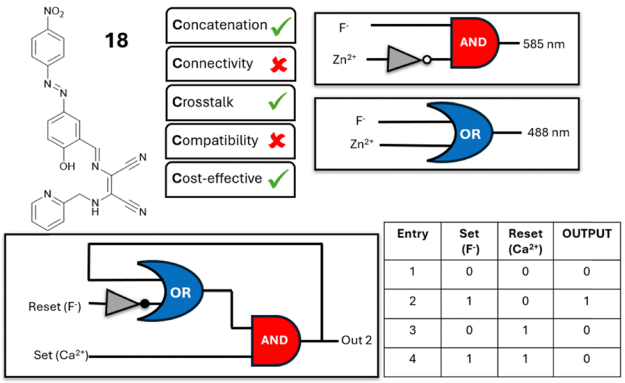



Fig. 14 Molecular logic gate **16** and **17**.




| Entry | Set ($F^-$) | Reset ($Ca^{2+}$) | OUTPUT |
|---|---|---|---|
| 1 | 0 | 0 | 0 |
| 2 | 1 | 0 | 1 |
| 3 | 0 | 1 | 0 |
| 4 | 1 | 1 | 0 |

Fig. 15 Molecular logic gate **18**.

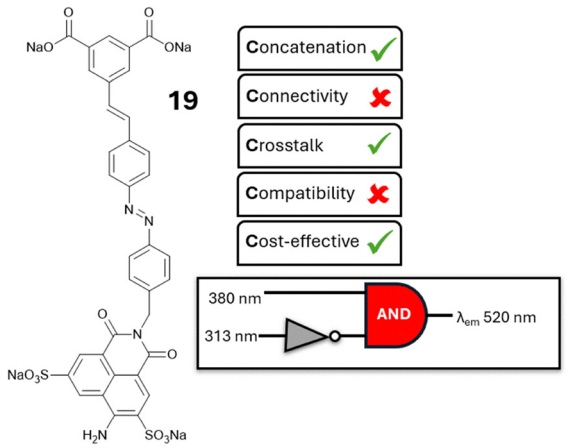



Fig. 16 Molecular logic gate **19**.

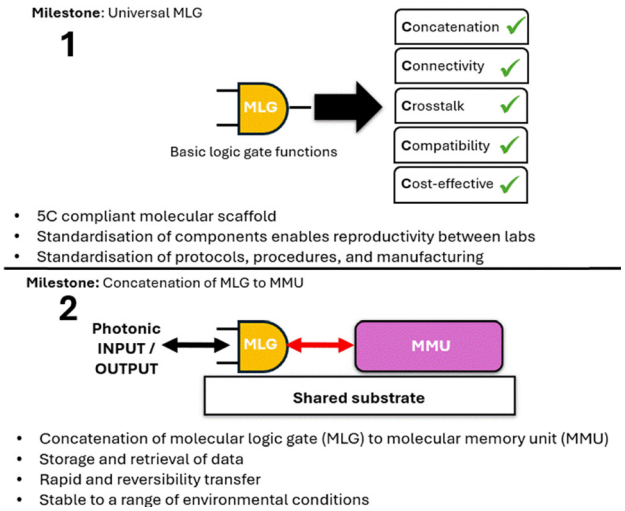
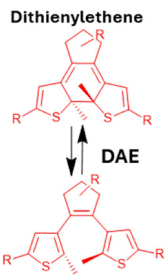
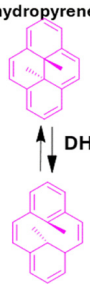
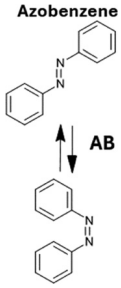


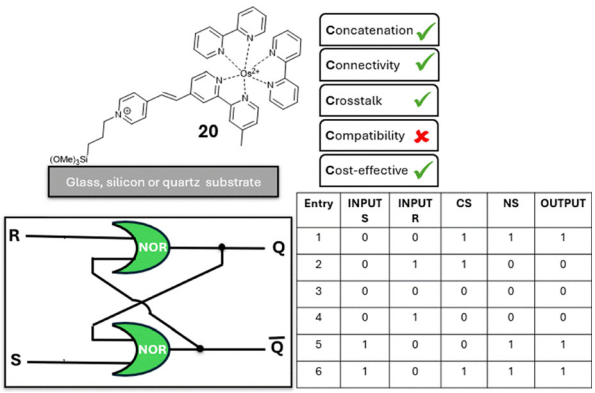

Fig. 17 The search for a universal molecular logic gate library (milestone one) and concatenation of molecular logic gates (MLG) with molecular memory units (MMU) (milestone two).

Fig. 15). When the Reset INPUT ($Ca^{2+}$) is present the OUTPUT reverts to O and the system is reset (entry 3 in truth table, Fig. 15). This process was repeated multiple times confirming reversible memory function. The use of molecular logic gates as memory units will be discussed further. This system demonstrates, concatenation, crosstalk and, cost-effectiveness meeting three of the five 5Cs.

A fully photonic azobenzene molecular gate was reported by Tian *et al.*, composed of a rotaxane consisting of a cyclodextrin macrocycle (just the logic gate unit is displayed (in Fig. 16 for clarity).[43] This system used 380 nm and 313 nm light as INPUT

Table 1 Summary of four molecular logic approaches

| | Dithienylethene | Spiropyran | Dihydropyrene | Azobenzene |
|---|---|---|---|---|
| |  |  |  |  |
| Advantages | Multiple logic gates<br>Well-established concatenation<br>High thermal and switching stability | Large signal response<br>Highly tuneable structure<br>Compatible with substrates | Large signal response<br>Robust switching<br>High thermal stability | Large signal response<br>Tuneable structure<br>Short synthesis |
| Disadvantages | Solution applications only<br>Slow photoswitching (μS)<br>Low signal-to-noise ratio | Limited concatenation<br>Low switching stability<br>Environmental sensitivity | Multi-step synthesis<br>Low photoswitching (μS)<br>Photochemical fatigue | Photodegradation<br>High crosstalk<br>Environment dependent |
| Emerging approaches | Visible light activation<br>Cascade logic circuits<br>Used as molecular logic and memory | Visible light activation<br>Supramolecular incorporation<br>Molecular logic and memory | Cascade logic circuits<br>Smart sensors<br>Multi-inputs (pH, voltage) | Visible light activation<br>Nanomaterial uses<br>Data storage |
| Conclusions | No single molecular structure meets all 5Cs criteria<br>Clear move away from UV light activation towards visible light as INPUT<br>Cascade devices to maintain signal strength<br>Combined use as logic gates and molecular memory | | | |




| Entry | INPUT S | INPUT R | CS | NS | OUTPUT |
|---|---|---|---|---|---|
| 1 | 0 | 0 | 1 | 1 | 1 |
| 2 | 0 | 1 | 1 | 0 | 0 |
| 3 | 0 | 0 | 0 | 0 | 0 |
| 4 | 0 | 1 | 0 | 0 | 0 |
| 5 | 1 | 0 | 0 | 1 | 1 |
| 6 | 1 | 0 | 1 | 1 | 1 |

Fig. 18 Molecular logic gate **20** as a substrate-bound SR latch.[57]

1 and 2 respectively and change in fluorescence emission at 520 nm as OUTPUT. Numerous other examples of combining azobenzene molecular gates with rotaxanes has been reported.[44] In summary, there are four leading contenders for fully photonic molecular logic gates: Dithienylethene,[45] such as **7–9**, Spiropyran[46] **10–13**, Dihydropyrene[47] **14–15**, and Azobenzene[48] **16–19**. Each scaffold has advantages and disadvantages (Table 1), with no one molecular structure meeting all five of the 5Cs. Emerging strategies for future work include shifting the photonic INPUT from UV to the visible and NIR range,[49] increasing signal strength *via* signal cascading,[50] and combined use for both logic and memory functions.

Photonic molecular logic gates are easily disturbed during readout, since the light used to probe them can trigger unwanted excitations, heating, or chemical changes.[45a,51] To address these challenges, researchers are developing non-destructive techniques and more resilient molecular designs. For example, approaches such as the incorporation of logic gates into supramolecular polymers,[52] logic gate-porphyrin hybrids,[53] and the use of unsymmetrical photochrome units are being explored.[54] These innovations are essential to ensure reliable, repeatable, and robust operation. The Roche electrolyte analyser highlights the commercial potential of transitioning molecular logic sensors to mass production (case study one).[55] We can now propose the first milestone on the path towards a molecular computer. We are yet to discover a single molecular scaffold that can replicate all the basic logic gate functions while meeting the 5Cs. The earliest electronic transistors were fabricated from germanium; however, once the superior properties of silicon were recognized, it rapidly became the material of choice.[56] This consolidation around a single platform concentrated research efforts on a single target and significantly accelerated progress. The identification of a universal molecular scaffold in molecular electronics would be similar, accelerating development while facilitating standardization and reproducibility across laboratories. The second milestone involves concatenating a molecular logic gate (MLG) to a molecular memory unit (MMU) to store and later retrieve data. This stored data must be reversible—allowing write, read, and deletion like the von Neumann architecture. We require compatibility between the MLG OUTPUT and MMU INPUT, all supported on an appropriate solid-state substrate. We will now examine recent developments in the field of molecular memory and potential solutions.

## Molecular memory and memristors

A key component of the von Neumann architecture[21] of general computing is a separate store of memory for the storage of programs and data. For molecular electronics to replicate this function, we require a form of short- and long-term reversible molecular memory. An early pioneering example by van der Boom *et al.* in 2010 based on an osmium polypyridyl complex **20** bound to a range of substrates (Fig. 18).[57] This system was based on an earlier reported osmium polypyridyl complex displaying several of

**Case study one: Roche electrolyte analyser**[55]

A prominent example of practical application of molecular logic gate concepts and photoinduced electron transfer (PET) sensing is the blood electrolyte analyser developed by A. P. de Silva in collaboration with Roche Diagnostics.[55] The device employs a PET-based INHIBIT logic mechanism, where biological cation binding ($Na^+$, $K^+$, $Ca^{2+}$) suppresses electron transfer, producing a fluorescence response. Commercialized between 2008 and 2013 with sales exceeding US $50 million, it enables rapid electrolyte quantification within 30 seconds, facilitating critical-care decision-making. de Silva received a Royal Society of Chemistry National Chemical Landmark plaque in 2024 in recognition for his contribution the field of molecular logic (Fig. 19).

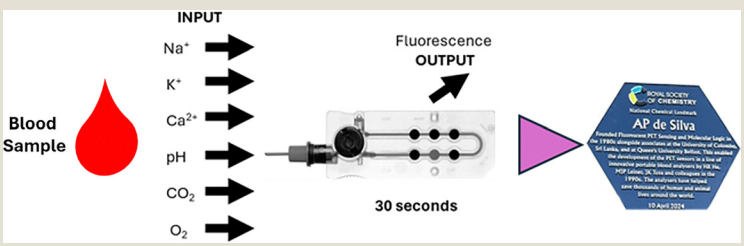



Fig. 19 The Roche blood analyser developed using the sensors from the de Silva group,[55] image reproduced ref. 55c with permission from Elsevier, copyright 2001.

the basic logic gate functions.[58] Substrate-bound **20** meets four of the five 5Cs and is an excellent example of organometallic compounds for molecular memory.

The concatenation of two NOR gates enabled **20** to store information *via* the Set/Reset (SR) latch mechanism. In this configuration, the osmium can exist in two different oxidation states, either $Os^{2+}/Os^{3+}$, with two INPUTs of $CO^{2+}$ (the set operation INPUT S) and $Cr^{6+}$ (the reset operation INPUT R). The OUPUT Q is adsorption intensity at 496 nm. For example, when the S or R INPUT are zero and the current state (CS) is 1 the next state (NS) is also 1 (entry 1 in Fig. 16). The system remembers the previous configuration. If the R INPUT is now set to 1 when the current state (NS) is 1, then the next state (NS) will be changed to 0 (entry 2). The system now contains no stored data (entry 3). In the presence of INPUT S when the current state (CS) is zero, the system stores this data as 1 in the next state (NS) (entry 5). Zhong *et al.* reported a similar molecular memory system in 2015 based on a diruthenium complex attached to a glass electrode (molecule **21**, Fig. 20).[59] This system used voltage at INPUT and a change in optical wavelength as OUTPUT with a similar SR latch configuration as in Fig. 18. While both **20** and **21** are pioneering examples of substrate-bound molecular memory, the use of metals and voltage as INPUT prevents the concatenation of photonic molecular logic and molecular memory units, a key requirement of milestone 2 (Fig. 17). The first fully photonic molecular report was in 2011 by the Andréasson and Pischel groups (molecule **22**, Fig. 21).[60] Molecule **22** operates *via* two INPUTs (clock at 532 nm and In at 1064 nm) both provided by an external laser. The OUTPUT is designated as fluorescence at 644 nm given, the designation Q current for the current state of the system and Q next for the next state of the system. A typical

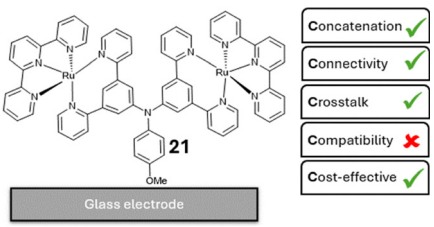



Fig. 20 Molecular logic gate **21**.[59]

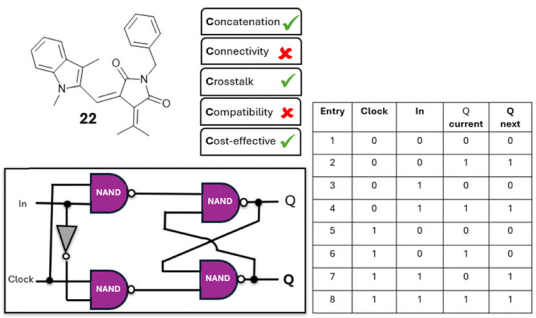



Fig. 21 Fully photonic molecular memory unit **22**.[60]

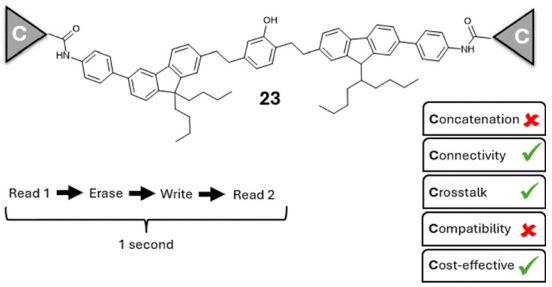



Fig. 22 Single molecule memristor **23**.[64]

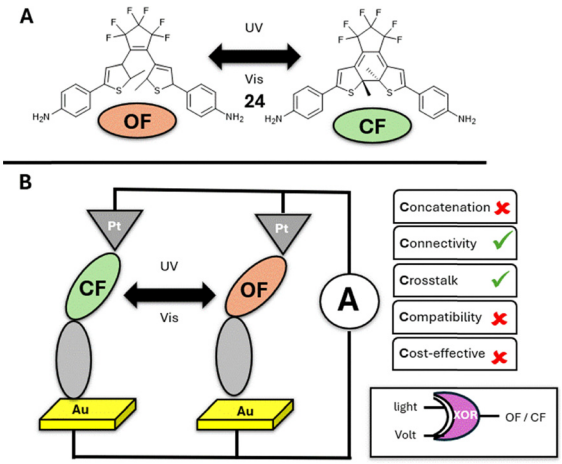



Fig. 23 Photonic memristor **24**, the diarylethene unit can photonically switch between open form (OF) and closed form (CF).[65]

operation is as follows: If both INPUTs are 0 and the current state of the system is 0 then the next state will also be 0 (entry 1 in table Fig. 21). If both INPUTs are 0 and the current state of the system is 1 then the system will remain in the 1 state for the foreseeable future (entry 2). If the longer wavelength light is 1 (In), then there is no change to the system and the current system state is maintained (if Q current is 0 Q next is 0 entry 3, or if Q current is 1, then Q next is 1, entry 4). The shorter 532 nm wavelength INPUT does not change the system if Q current is zero (entry 5); however, it will trigger the system to flip to the 0 position if the Q current is 1 (entry 6).

This system was cycled ten times without loss of operation.[60] The authors stated that the barrier of INPUT/OUTPUT heterogeneity limiting the concatenation of similar devices could be overcome with this approach. The multi-directionality of the emitted light is a potential future concern. Nanomaterials as a possible solution to this concern and will be discussed later. Molecule **22** clearly demonstrates that fully photonic molecular memory is possible. Alongside the short-term storage of data **20–22** provides, we require a form of long-term store of data. Memristors are a recent and promising potential solution. The term memristor (composed of the words memory and resistor) was proposed by Leon Chua in 1971,[61] with the first reported memristor by HP labs in 2008.[62] Since then, a multitude of reported materials have been discovered, with memristors often

**Case study two: Heisenberg molecular overdrive**[68]

The first commercial molecular electronic device was available in 2017 specifically for the music industry.[68] The Heisenberg molecular overdrive electric guitar pedal provides the distinct electric guitar growl by passing a voltage across a molecular junction composed of azo compounds (Fig. 24A). These molecular junctions were produced on a SIM card substrate (Fig. 24B). While Nanolog Audio, Inc. are no longer manufacturing these devices, they are in still in use and with numerous online review available.[69] This highlights that molecular electronics can transition from the laboratory to commercial devices.

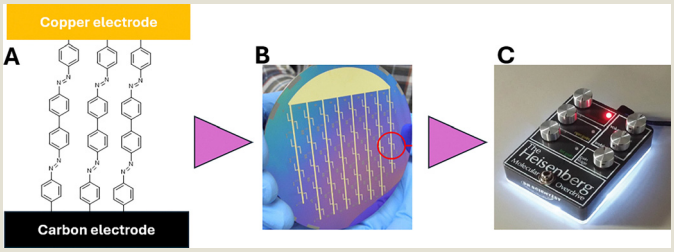



Fig. 24 The molecular junction responsible for the devices function (image A), the mass production of SIM cards (image B) image reproduced from ref. 68*a* with permission IOP Publishing, copyright 2016 and the final commercialised product (image C), image reproduced from ref. 68*b* with permission ACS, copyright 2016.

cited as a material to deliver beyond Moore's law.[63] In 2022, Guo *et al.* reported the first single-molecule memristor, **23**, between two graphene electrodes (Fig. 22).[64] On application of voltage, the OH group on **23** can switch between *ortho* and *para* positions, enabling the non-volatile storage of data in two different molecular configurations. These states can be reversed multiple times enabling the read, erase, write, and read operations within a second.

While **23** is an excellent example of non-volatile molecular memory attached to a substrate, the use of voltage as INPUT limits the ability to concatenate this type of MMU to a photonic MLG. An alternative memristor reported by Lacroix *et al.* in 2025 is based on a diarylethene dimer held between two electrodes which used light as INPUT (Fig. 23B).[65] System **24** is the first reported photonic molecular memristor, which also acts as a XOR gate and is a pioneering example of combing molecular logic and molecular memory. The diarylethene unit can flip between open form (OF) and closed form (CF) on application of UV or visible light (Fig. 23A). The assembly of a dimer of diarylethene **24** between gold and platinum electrodes enables the non-volatile storage of data. The system can alternate between OF (0 bit) and CF (1 bit) form in under 2 seconds. In summary, there are currently three approaches to molecular memory: organometallic compounds[66] bound to substrates **22-21**, fully photonic[67] solution-bound molecules **23**,[60] and molecular break junction-bound molecules **23–24** (Fig. 23).

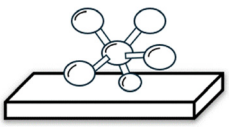
Each approach has its advantages and limitations (Table 2), but all clearly demonstrate the short and long-term storage of data on the molecular level. The first commercially available device incorporating molecular electronics was the Heisenberg molecular overdrive (case study two).[68,69] After navigating multiple manufacturing challenges, this device was realized, offering a clear example of how molecular computers can be built from the "bottom up". The third critical milestone on the road to a molecular computer is the integration of multiple molecular logic and memory units onto a single substrate (Fig. 25). Transitioning from solution to solid-state is vital to enable the organised arrangement of multiple molecular units onto a single device. Recent developments in nanomaterials are providing valuable examples in this regard.

## Molecular interconnects and nanoarchitectonics

The next step in developing molecular computing systems is the integration of discrete molecular components into functional circuits. Nanoarchitectonics focuses on designing and assembling devices from individual molecules and nanomaterials, and nanostructures.[70] Nanomaterial interconnects will be pivotal to connect components and ensure coordinated function. Among these, nanowires, nanotubes, and nanorods are particularly critical (Fig. 26). The use of microtubes in the photonic industry as waveguides is well-established,[71] and this is providing a valuable resource for the attachment of molecular electronics to substrates.

The example of spiropyran **13** on a polydiacetylene microtube has been previously discussed (Fig. 11).[36] A particularly advantageous property of polydiacetylene microtubes is the ability to transfer polarised light, which could be utilized to prevent crosstalk between adjacent microtubes. Viologen **25** was attached to polydiacetylene microtubes *via* click chemistry and displayed AND and INHIBIT logic functions (Fig. 27).[72] The concatenation of two INHIBIT gates was established, confirming **25** met four of the 5Cs challenges. The authors highlighted that this system displayed polarization and would be a valuable platform for future optical computing applications. Polydiacetylene microtubes are particularly useful substrates for sensing applications. Nanowires are related to microtubes however while microtubes are hollow, nanowires contain a solid core. One of the earliest reports of nanowires displaying logic functionals was reported by Jussila *et al.* in 2018 composed of a InP

Table 2 Molecular memory summary

| | Organometallics | Photonic molecules | Molecular memristors |
|---|---|---|---|
| |  |   |  |
| Advantages | • Multiple substrate bound examples<br>• Well-established chemistry<br>• Low-cost materials | • Fully photonic INPUT/OUTPUT<br>• Lightspeed signalling<br>• Low energy use | • Low energy use<br>• High stability<br>• High density memory storage |
| Disadvantages | • Metal INPUT only<br>• Limited concatenation<br>• $O_2$ and moisture sensitivity | • Limited substrate-bound examples<br>• High crosstalk<br>• Limited examples reported | • Limited scale-up<br>• Complex fabrication<br>• Environmental sensitivity |
| Emerging approaches | • Multi-level memory *via* redox states<br>• Duel redox and light INPUT<br>• Integration with nanomaterials | • Multiple wavelengths utilised<br>• Integration with nanomaterials<br>• Plasmonic enhancement | • High density memory storage<br>• Integration with nanomaterials<br>• Real-time monitoring *via* TEM |
| Conclusions | – Move towards fully photonic devices for rapid and reversible INPUT/OUTPUT<br>– Recent examples of concatenation of molecular memory with logic gates established<br>– Integration with nanomaterials to improve performance (signal strength, environmental robustness) | | |

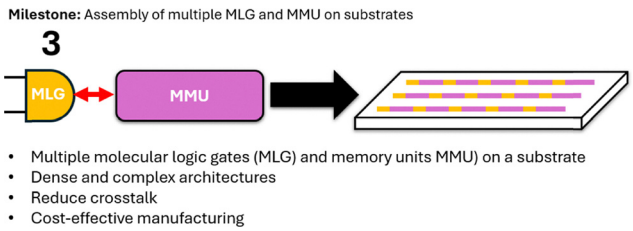



Fig. 25 Milestone three, the functional assembly of multiple molecular components onto a single substrate.

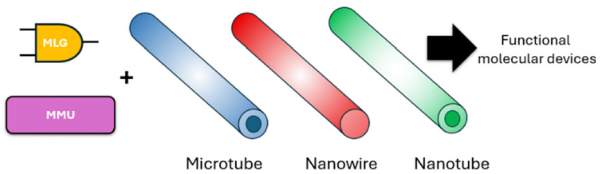



Fig. 26 Use of 1D nanomaterials for molecular interconnects.

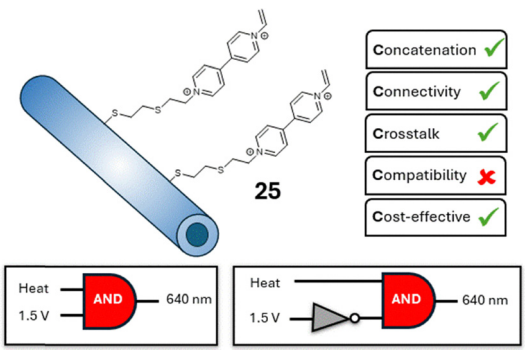



Fig. 27 Viologen **25** bound to Polydiacetylene.[72]

and AlGaAs nanowire network **26** (Fig. 28).[73] There was no chemical modification to the nanowire surface, yet regions at which the nanowires meet were confirmed to display both NAND and NOR logical functionality. This system met three

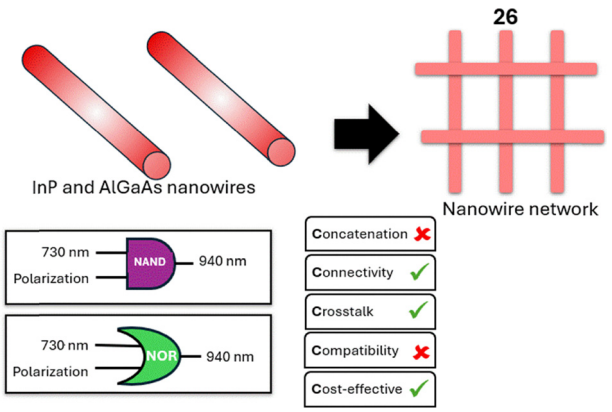



Fig. 28 Nanowire network **26**.[73]

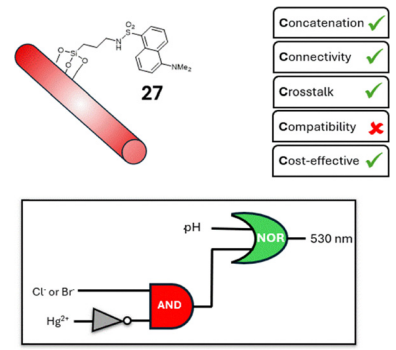



Fig. 29 Nanowire with **27** on the exterior.[74]

out of the five 5Cs. Further reports of nanowire displaying logic functionality have been reported, for example **27** (Fig. 29).[74]

Lee *et al.* reported dansyl **27** grafted to silicon nanowires which displayed multiple logic gates confirming four of the 5Cs.[74] One attractive feature of nanowires is their high conductivity properties, which have made them particularly useful in the flexible electronic industry, particularly for wearable human-machine interfaces.[75] There is currently great interest

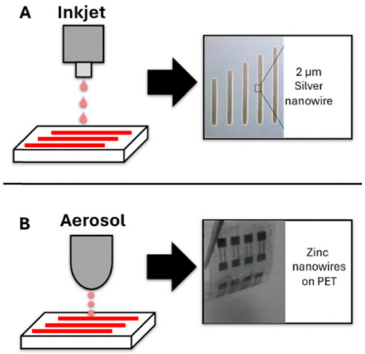



Fig. 30 3D printing of nanowires, images reproduced from ref. 78 and 79 with permission from ACS, copyright 2015, and RSC, copyright 2013 respectively.

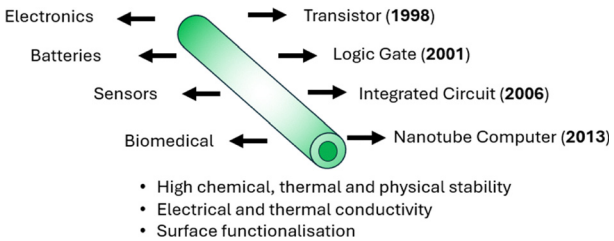



Fig. 31 Nanotube summary.

in switching from batch to continuous flow synthesis of nanowires due to their widespread application in emerging industries.[76] This is likely to reduce production costs as the uptake of nanowire-based applications increases, ensuring nanowires meet the cost-effective criteria of the 5C. Numerous reviews are available for printable electronics;[77] here, we provide an example of inkjet[78] and aerosol[79] of 3D printing of nanowires (Fig. 30A and B). Coleman *et al.* printed silver nanowires on poly(ethylene terephthalate) (PET) surfaces with 1–10 mm line widths.[78] Pan *et al.* printed zinc octaethylporphyrin nanowire on a PET substrate *via* aerosol printing with nanowire diameters of 200 to 400 nm, and average lengths up to 200 mm.[79] Carbon nanotubes were first discovered in 1998 by Sumio Iijima[80] and have found a multitude of applications, including batteries, sensors, and biomedical applications.[81] The use of nanotubes in electronics is particularly interesting due to the high chemical, thermal,

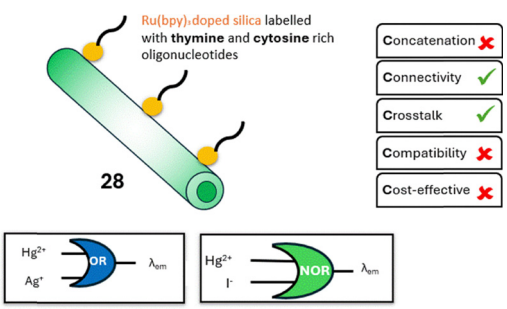



Fig. 32 Multiwalled carbon nanotube (MCNT) with $Ru(bpy)_3$ silica and thymine and cytosine oligonucleotide functionalisation.[88]

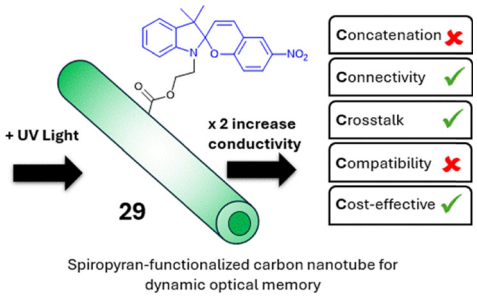



Fig. 33 Spiropyran **29** bound carbon nanotube.[89]

and physical stability, alongside high electrical conductance.[82] The surface of the nanotube can also be functionalised *via* a variety of methods (Fig. 31).[83]

The first reported carbon nanotube (CNT) transistor[84] was in 1998 shortly followed by the first logic gate in 2001.[85] Integrated circuits,[86] and then the first nanotube computer,[87] demonstrate the high interest in this nanomaterial. Ge *et al.* reported a multiwalled carbon nanotube with thymine and cytosine functionalisation, which displayed OR and NOR logic gate properties in the presence of different metals (**28** in Fig. 32).[88] Thymine-rich oligonucleotides specifically bind $Hg^{2+}$ ions whereas, cytosine-rich units will bind $Ag^{+}$. The addition of both onto the surface of a nanotube enables logic functionality such as OR and NOR gates. This system displayed two of the five 5Cs, the use of metal INPUT prevents the concatenation of multiple units, and the use of oligonucleotide is not cost-effective. Zaumseil *et al.* reported a spiropyran bound to semiconducting single walled carbon nanotubes which on exposure to UV light results in the spiropyran converting to the merocyanine form increasing conductivity (**29** in Fig. 33).[89]

This system acts as an optical memory, it can remember UV exposure until a reset signal (heat) is applied. This is an example of the hybridization of photochromic molecules and nanomaterials for molecular memory. Carbon nanotubes have also been functionalised with dithienylethene, for example, **30** reported by Aida *et al.* (Fig. 34).[90] In the presence of UV light, the dithienyleene can flip from open to closed form, resulting in an increase in the conductivity of the nanotube. In summary, nanotubes have been developed for molecular electronic

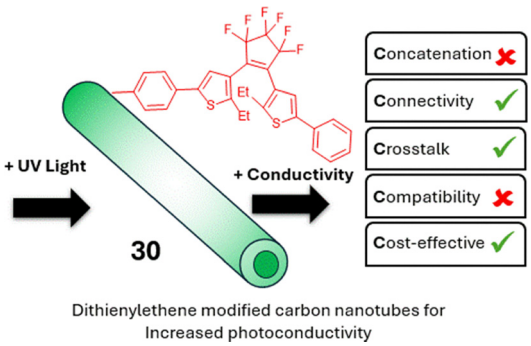
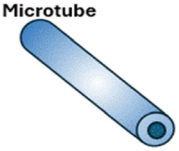
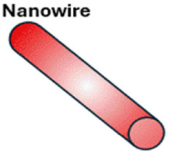
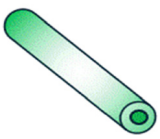



Fig. 34 Dithienylethene **30** bound to carbon nanotube with increased conductivity on exposure of UV light.[90]

Table 3 Nanomaterials summary

| | Microtube | Nanowire | Nanotubes |
|---|---|---|---|
| |  |  |  |
| Advantages | • Use as waveguides to reduce crosstalk<br>• Surface functionalization with logic gates<br>• Low-cost materials | • Ease of synthesise (SAMs, VLS)<br>• Surface functionalization with logic gates<br>• High electrical conductivity | • Well-established chemistry<br>• Multiple application in electronics<br>• Large-scale fabrication established |
| Disadvantages | • Poor mechanical stability<br>• Limited scale-up fabrication<br>• Batch-batch variability | • Poor thermal stability<br>• Low fabrication yield<br>• Aggregation issues | • Poor thermal stability<br>• Integration and alignment challenges<br>• High contact resistance |
| Emerging approaches | • Template-assisted growth<br>• Conductive polymer blends<br>• 3D architectures | • Core-shell nanowires<br>• Directed self-assembly<br>• CMOS integration | • Metal-nanotube junctions<br>• Polymer-nanotube composites<br>• Nanotube based electronic devices |
| Conclusions | – Improvements in mass production (reduce batch-batch variability and reduce costs)<br>– Use of multiple materials to fine-tune properties to improve performance<br>– Organised surface assembly and development of functional devices (case study three) | | |

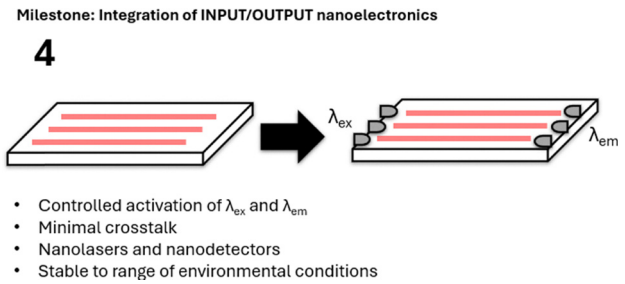



Fig. 35 Integration of nanoelectronics.

purposes but mainly for the use of transistors and the assembly of integrated circuits and nanocomputers. The surface modification of nanotubes has been widely reported however, there are limited reports of the attachment of molecular logic gates to the surface. The majority of studies have involved the use of photochromic molecules to enhance the conductive properties of the nanotube itself. A comparison contrasting the advantages and disadvantages of each nanomaterial is in Table 3.

The development of the carbon nanotube (CNT) computer (case study three) demostrates nanomaterial potential in new computing paradiagms. We can now propose our fourth milestone on the road towards a molecular computer, the integration of nanoelectronics with substrate-bound molecular components (Fig. 35). We require a method of controlling the INPUT/OUTPUT signals of the molecular logic and memory units with the discovery of the nanowire laser in 2001 a promising solution (Fig. 37).

## INPUT/OUTPUT

The utilisation of light as both INPUT and OUTPUT for molecular logic gates (MLGs) and molecular memory units (MMUs) has been discussed, we now require a method of transmitting and receiving these inputs on the molecular scale. The invention of the LASER (light amplification by stimulated emission of radiation) in the 1960s transformed multiple areas, enabling high precision spectroscopic techniques, medical use in surgery and data communication technologies.[91] Reduction in size of the laser

**Case study three: a carbon nanotube (CNT) computer**[87]

The world's first carbon nanotube (CNT) based computer, nicknamed "Cedric", was reported in 2013 capable of performing basic operations.[83] Significant technological challenges were overcome to achieve this, including alignment of the CNTs on the quartz substrate with greater than 99.5% accuracy. In 2019 a more advanced version, RV16XNano, was reported which could run basic computer programmes (Fig. 36).

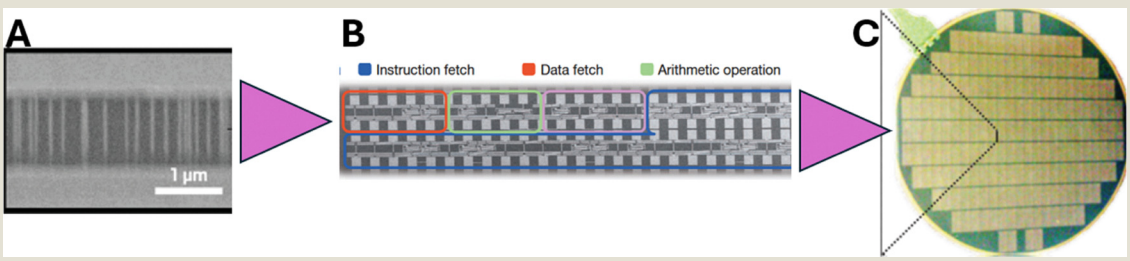



Fig. 36 The assembly of aligned CNTs (panel A), configuration of the IC (panel B) and the mass-produced final unit (panel C), image reproduced from ref. 87 with permission from NPG, copyright 2013.

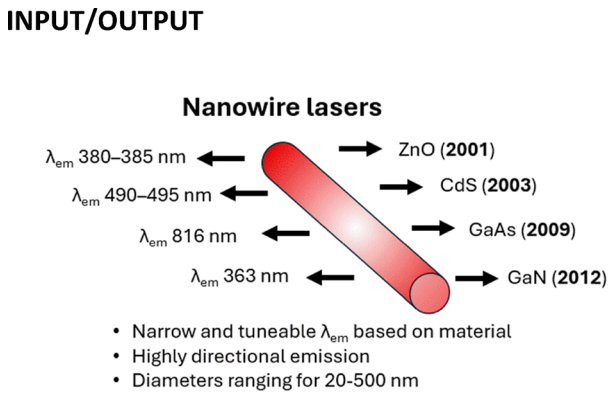



Fig. 37 Nanowire lasers reported between 2001–2012.

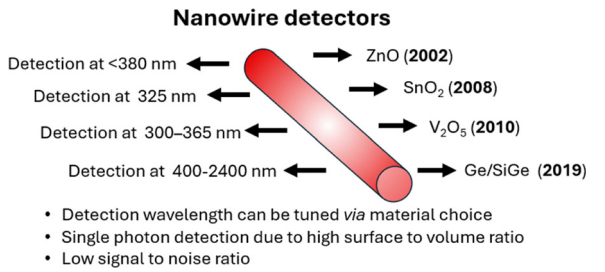
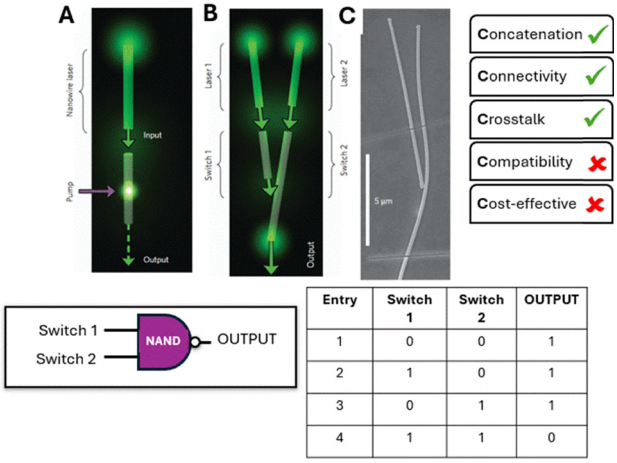



Fig. 38 Selection of nanowire detectors reported between 2002–2019.

enabled the transmission of information in the form of light *via* fibre optic cables, realizing global communication and enabling the internet. Further laser miniaturization unlocked on-chip lasers which transformed the photonic industries.[92] The first reported nanowire laser was reported by Yang *et al.* in 2001, based on a ZnO nanowire.[93] The choice of nanowire material enables wavelength of emission ($\lambda_{em}$) selection (Fig. 38), which, when coupled with the high directionality and nanoscale dimensions, provides a nanoscale toolbox of electronic components. A selection of reported nanowire laser applications includes the use as intracellular probes and biosensors, quantum information sensing, and hybridisation with plasmonic materials.[94] Nanowire lasers can deliver precise and controlled transmission of photons to molecular logic gates. Alongside their use as nanolasers, Yang *et al.* reported the use of ZnO nanowires as UV photodetectors in 2002.[95] The choice of material for the nanowire enables fine-tuning of the detection wavelength. High surface-to-volume ratio enables very high sensitivity with the ability to detect single photons.

Since the initial nanowire detector in 2002, a variety of other materials have been discovered (Fig. 38).[96] Typical applications for nanowire detectors include use in quantum technologies, biological sensing of DNA and viruses, chemical sensing of single molecules, and their use in optical switching in photonics.[97] A pioneering example of the use of nanowires as optical switches was reported by Agarwal *et al.* in 2012 and demonstrated the first CdS nanowire NAND gate on a silicon substrate (Fig. 39).[98] Upon excitation at 457.9 nm with an $Ar^+$ laser, signal is transmitted through a gap of approx. 460 nm to the CdS nanowire switches 1 and 2. With no $Ar^+$ excitation, this corresponds to entry 1 in the




| Entry | Switch 1 | Switch 2 | OUTPUT |
|---|---|---|---|
| 1 | 0 | 0 | 1 |
| 2 | 1 | 0 | 1 |
| 3 | 0 | 1 | 1 |
| 4 | 1 | 1 | 0 |

Fig. 39 CdS nanowire NAND gate, images reproduced from ref. 98 with permission from NPG, copyright 2012.

truth table for a NAND gate (Fig. 39). When the $Ar^+$ excitation is focused on switch 1 only, this represents entry 2, whereas when on centred switch 2 entry 3 applies. When $Ar^+$ excitation is present in both switches, all transmission is ceased and entry 4 is applicable. This example clearly demonstrates the usefulness of nanowires for the transmission of light and the performance of logical functions.

Recent advances in the large-scale handling of nanowires with high precision and reproducibility,[99] and construction of highly organised nanowire networks, demonstrate this is the material of choice for future molecular electronic development.[100] The fifth and final milestone towards a molecular computer is the integration of a molecular integrated circuit (MIC) with traditional silicon-based electronics (Fig. 40). The ability to merge two distinctly different approaches to computing into a functional device will firmly establish molecular computing as a strong successor to the silicon IC. The integration of photonic integrated circuits with traditional silicon-based ICs is providing significant improvements to datacentres. This demonstrates that hybridisation is possible. The "Hello world" programme is a well-established test to determine if a system can run basic programming commands and would be an excellent test for milestone five. The Roswell molecular electronics chip (Fig. 41) demonstrates the valuable application of molecular electronics in the healthcare industry (case study four).[101] To replicate this significant achievement in pursuit of the world's first molecular computer, we require the

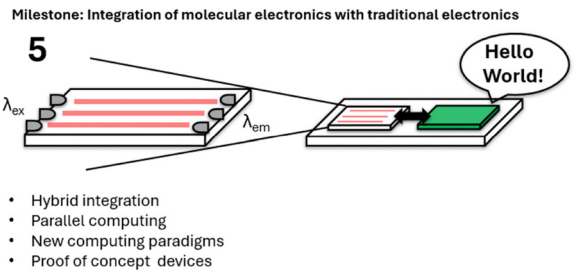



Fig. 40 Hybrid integration of molecular electronics with traditional electronics (in green).

**Case study four: Roswell molecular electronics chip**[101]

The world's first molecular electronics chip features a sensor array with more than 16 000 sensors, each built around a molecular wire conjugated to a specific probe of interest (Fig. 41).[57] When a target molecule binds, it produces a measurable change in electrical resistance at the single-molecule level, enabling real-time readout. This platform delivers label-free detection across a wide range of analytes. Importantly, the chips are fabricated using standard semiconductor manufacturing processes, making large-scale production efficient and cost-effective. This technology stands as a landmark example of how molecular electronics can drive the next generation of healthcare innovations.[58]

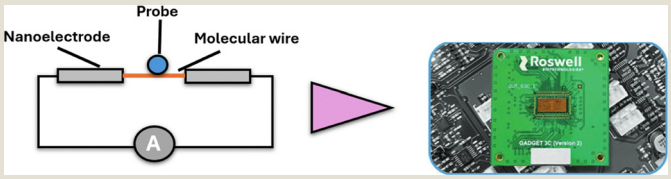
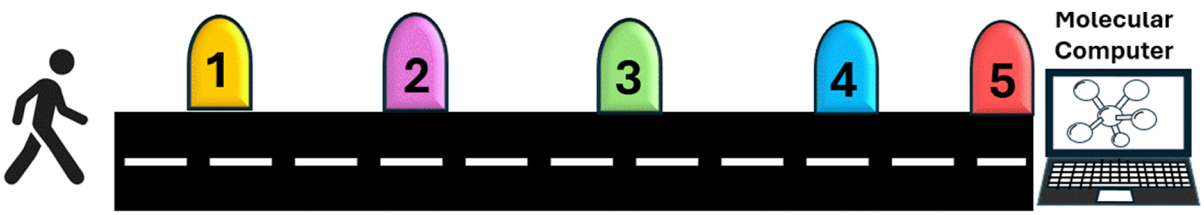



Fig. 41 The Roswell molecular electronics chip, image reproduced from ref. 102 with permission from Wiley, copyright 2023.

| | |
|---|---|
| **Strengths** | • Parallel computing and a paradigm shift for generations to come<br>• Low power usage and heat generation provide huge energy efficiency<br>• Ultra-high-density processing and data storage beyond Moore's Law |
| **Weaknesses** | • Unable to design circuits from the "bottom-up"<br>• Complex device fabrication makes cost prohibitive- unviable commercially<br>• Unable to replicate the "bottom-up" approach of nature; "top-down" prevails |
| **Opportunities** | • Decentralised computing manufacture reduces geopolitical tensions<br>• Biological applications unsuitable for silicon-based electronics unlocked<br>• Neuromorphic computing enabling advanced AI and ML applications |
| **Threats** | • Competing technologies reach maturation before molecular electronics<br>• No standardisation of methods and techniques- field stagnates<br>• Low uptake of new technology- no mass adoption |

Fig. 42 SWOT analysis for molecular computing.




| | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| **Specific** | **1**: Develop a universal MLG | **2**: Concatenate MLG - MMU | **3**: Substrate MLG-MMU | **4**: Nanowire integration | **5**: Hybrid prototypes |
| **Measurable** | Must display all basic logic gate functions | Reversible storage and retrieval of data | Multiple molecular units configured on a single substrate | Reversible and rapid INPUT / OUTPUT under range of conditions | Confirm molecular and silicon electronics can coexist |
| **Attainable** | Numerous chemical scaffolds are available | Proof-of-concept established | Case studies 1-4 confirm substrate bound molecular devices possible | Nanotube computer confirms this can be achieved | Photonics industry confirms hybridisation is possible |
| **Relevant** | Enables standardisation across laboratories and focus efforts | Essential to enable general purpose molecular computing | Critical to move from solution to solid-state devices | Cost-effective mass production is essential to compete with existing technologies | Confirms molecular electronics can compete with current technologies |
| **Timely** | First objective 2-5 years | Second objective 5-8 years | Third objective 8-10 years | Forth objective 10-15 years | Fifth objective 15-20 years |

Fig. 43 SMART goals for the five milestones.

convergence of multiple technologies to solve a single problem. By clearly emphasizing the milestones ahead, we focus and accelerate their development. The four case studies highlighted within demonstrate the tangible benefits to society molecular electronics offer.[102]

## Conclusions and future directions

Silicon-based transistors have powered the technological revolution for the past seven decades, despite valiant efforts to prolong silicon; its limitations are increasingly clear. Continued miniaturization of silicon transistors will shortly reach a scientific, technological, and economical roadblock. To sustain the progress demanded by society, new paradigms are needed. Molecular electronics, first envisioned in the 1970s, is experiencing a resurgence as a promising successor to traditional computing. Significant advances have already been made in individual molecular logic components—including logic gates, memory components, interconnects, and architectures. The next critical step is cohesive integration of these components into functional molecular devices from the "bottom-up". Several successful molecular electronic case studies demonstrate progress already achieved. The final destination for molecular electronics is development of the world's first molecular computer, a goal now well within reach.

As societal demand for computational power continues to grow exponentially, advancement towards molecular-scale devices is inevitable. There are still significant obstacles ahead, a SWOT (Strengths, Weaknesses, Opportunities, and Threats) analysis provides further in-depth analysis on the path ahead (Fig. 42). We have identified five milestones on this journey ahead, and establish SMART (Specific, Measurable, Attainable, Relevant, and Time-bound) goals for each one (Fig. 43). Each SMART goal is designed to critically analyse the path ahead and how to meet the challenges head on. Although the journey ahead may seem complex with many obstacles to overcome, it mirrors the challenges faced by the pioneers of the 1950s who developed the first integrated circuit—an invention that redefined the modern world. Several obstacles have already been overcome for case studies 1–4 to reach commercial success. The development of a molecular computer is likely to follow a similar trajectory. Molecular electronics represents the final frontier in miniaturisation, realising Richard Feynman's vision that there is indeed "plenty of room at the bottom".[18]

## Author contributions

Alexander Ciupa authored the manuscript.

## Conflicts of interest

There are no conflicts to declare.

## Data availability

No primary research results, software or code have been included and no new data were generated or analysed as part of this review.

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