



CHEMPUTATION

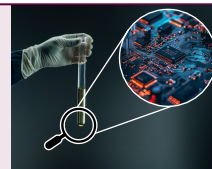
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Playing Doom on a Molecular Computer

D. Guy^A, M. Chief^B and G. Schlönc^{C*}**Abstract: It runs Doom!**

Specific: We report a quantum leap forward in the field of nanocomputing, with the development of a fully-operational molecular computer. Our device, the DORF4000, contains discreet processing, storage and signal input/output domains, all in a volume smaller than the tip of a pin. To benchmark the DORF4000's performance, we demonstrate that it is capable of running the video game Doom (1993).



Introduction

There are so many impending calamities queueing to topple our civilisation that it's becoming quite tricky to keep track of them all. News broadcasts sound like half-speed commentary of a global Grand National: "...and its Climate Change in the lead, Climate Change followed by Nuclear War, Pandemic creeping up on the outside there, Dying Bees is falling behind now...". Amidst all this commotion, the imminent failure of Moore's law has been almost completely overlooked. Moore's law, first posited in 1965, states that the number of transistors in computer chips will double every two years. This has largely held true, but scientists are approaching physical limits to the extent by which transistors can be downsized. That doesn't sound so bad, but the reader should recall that if our computer games stop getting progressively better, we'll actually have time to think about all the other crises we're facing.

If we can't make conventional transistors any smaller, the obvious solution is to start as small as one can, and work in the opposite direction. Significant research efforts have been devoted to developing single-molecule transistors and suchlike, but so far little of practical use has emerged. Rather than an incremental improvement in transistor design, we report the development of a functioning molecular computer: the DORF4000.

One of the most important things computers are used for is gaming. Doom (1993) is the father of first-person shooters, and one of the most influential games of all time. Thanks to its simple code, bored programmers have ported it onto almost every device with a screen, including treadmills, cameras, vapes, pregnancy tests, calculators and microwaves.¹ As such, we selected "the capacity to run Doom" as the benchmark for success of our molecular computer.

Design

In the process of collapsing an entire computer into a single molecule, it was necessary to eschew several features of conventional computers, such as wireless connectivity, dedicated graphics processing, cooling and a power supply. Instead, our device required a means of receiving external signals and transmitting an output, a processor, and some form of chemical memory capable of encoding an operating system and the game data (Figure 1). We envisioned a highly simplified device, with less computing power than a Breville Smart Toaster, but more than a Samsung Galaxy A13.

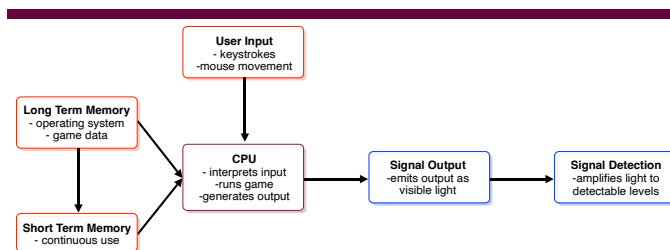


Figure 1: A schematic overview of our molecular computer.

User Input

Developing a molecular keyboard was the first challenge we confronted. We initially experimented with a mechanical-style keyboard, but we discovered that our fingers were too big to press the keys selectively, by about seven orders of magnitude. An essential feature of all gaming keyboards is that they light up with pretty colours (Figure 2B). This observation inspired our strategy. We designed the ChromeBoard™: a molecule that emits electrical signals in response to different colours of light, instead of in response to pressing keys (Figure 2A).

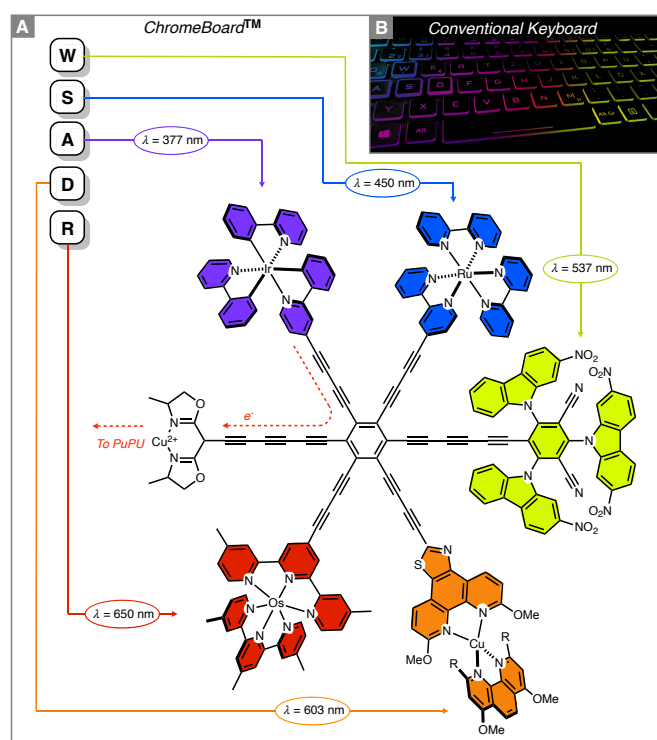


Figure 2A: Our novel molecular keyboard. When illuminated by a laser at one of five wavelengths, an electron is ejected from the appropriate photocatalysts, and transferred to processor via the alkynes. **2B:** A conventional gaming keyboard.

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We accomplished this by tethering five photocatalysts to a benzene scaffold with alkynes. When one of these photocatalysts is excited by a photon of the appropriate wavelength, an electron is ejected, and travels to the CPU via the alkyne linkers. Because photoactive molecules have broader-than-ideal absorption profiles, it was not possible to fit a full QWERTY keyboard into our ChromeBoard™, and we had to make do with five keys. As such, we had to make some compromises when it came to mapping keys in-game:

- W (537 nm): move forward
- S (450 nm): look left
- A (377 nm): strafe left
- D (603 nm) shoot
- R (650 nm): interact

For instance, shining blue light on the ChromeBoard™ will make Doomguy look left, but there is no way to make him look right, except by turning 270° the other way. Unfortunately, if two photocatalysts are activated simultaneously, the entire molecule decomposes into the “blue sludge of death”.

CPU

In the design of our molecular processing unit, we treated a conventional CPU as a large array of binary on-off switches (transistors). Single-molecule magnets such as terbium complex **1** have attracted attention in this space, as their inherent magnetism (spin up/down) could potentially be used to store information. As yet, no systems have been reported incorporating more than a few such magnets into a single unit. A CPU with three transistors would result in an unacceptably laggy gameplay experience, so we devised a strategy to link multiple molecular magnets. We began with benzene hexanitride, which we reduced with KC_8 in the presence of plutonium(III) chloride to generate sandwich complex **3**. This complex exhibits molecular magnetism, thanks to the single-occupancy of the ξ^{msg} molecular orbital. Then we simply co-crystallised **3** with six equivalents of PdCl_2 to generate a metal inorganometallically-linked framework or “MILF”.² We isolated

a crystal containing 486 units of **3** which we used as the Plutonium Processing Unit or “PuPU” in our molecular computer. As patents are pending on the workings of the PuPU, we cannot detail its mechanism at this time, so just trust us that it works.

Memory

To run Doom, our molecular computer required a system to store the game’s code within its structure, alongside an operating system such as MS-DOS. These two files constitute about 18 billion bits of information, which is much more than our PuPU can accommodate. Thankfully, nature has already devised a system for encoding databases of this magnitude, in the form of DNA. The human genome consists of approximately 3 billion base pairs, in which each base pair is either an adenine-thymine (AT) or cytosine-guanine (CG) couple. It thus proved to be a relatively simple task to transpose the binary code of MS-DOS and Doom (0’s and 1’s) into the binary code of life (AT’s or GC’s). It was somewhat harder to find a supplier to create our custom DNA sequence. In the end, we had to do it ourselves by splicing 120 base-pair segments into the genome of the lesser-spotted field potato (*Batatas micromaculosus*), one at a time. This body of chemical information constitutes the hard-drive of our molecular computer, though given the flexible nature of DNA, its actually closer to a floppy disk (Figure 2B).

As even chemistry graduates know, computers need short term memory in addition to hard-drive space. Again, we co-opted nature’s cellular machinery to replicate this technology *in molecula*, by incorporating several RNA polymerases into our computer. When the appropriate transcription factors are added, these enzymes convert the relevant sections of the game’s code into short, rapidly accessible fragments of mRNA. These packets of mRNA are then read by a series of ribosomes, tethered to the PuPU. The ribosomes were engineered such that electrons were produced (in place of peptides), which were transferred to the PuPU (*vide infra*). We suggest this form of information transfer be called “Ribonucleic Acid Memory” or RAM for short. RAM exhibits a generally high degree of fidelity, although it is vulnerable to attack by viruses.

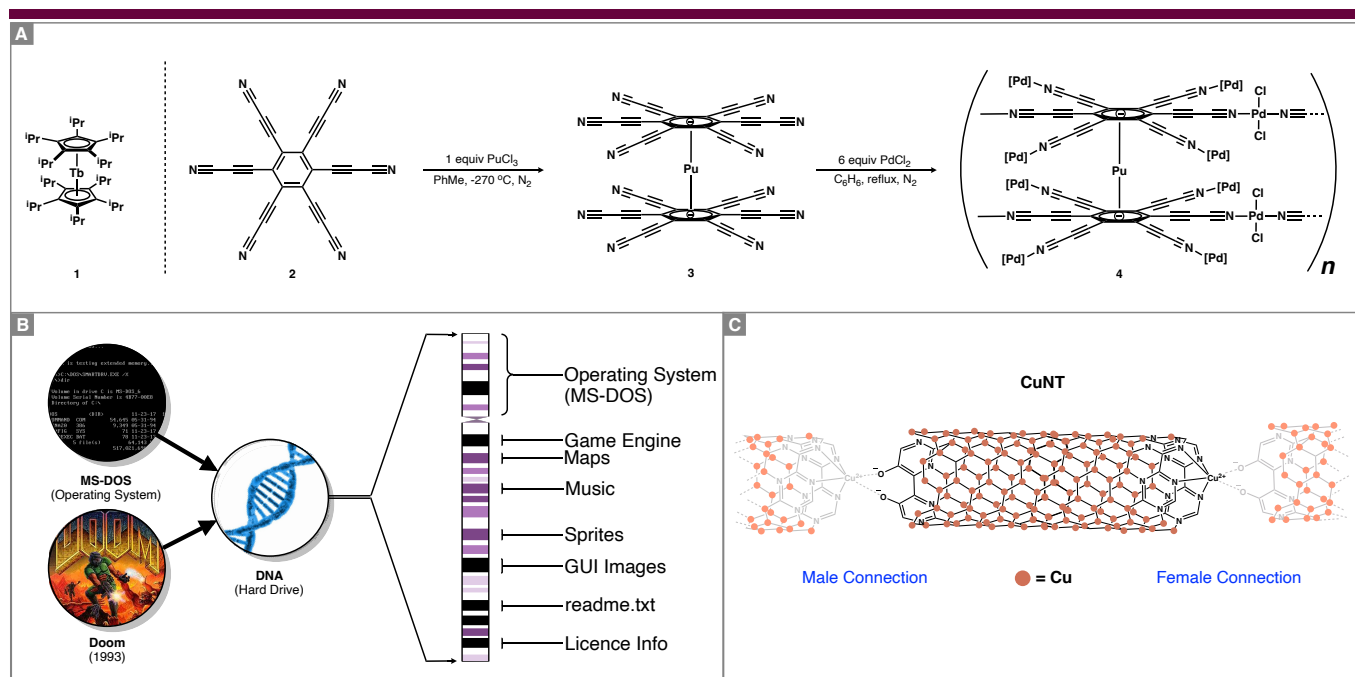


Figure 2A: An example of a conventional single-molecule-magnet (**1**), and the synthesis of our novel plutonium-MILF, **4**. We employed a crystal containing ~486 repeating units of **4** as our molecular plutonium processing unit (PuPU), in which each metal centre behaves as a magnetic transistor. **2B:** An overview of the file directory for our molecular computer. **2C:** Modified copper nanotubes (CuNTs) were developed to serve as self-assembling wires between the components of the DORF4000.

Wiring and Cable Management

Macroscopic computers predominantly use copper wiring, either in the form of cables or printed circuit boards. However, when we attempted to wire our molecular computer together with 650-gauge copper thread, the heat from the soldering iron denatured the hard-drive. Evidently, we required a truly molecular solution. The answer was provided to us by a fantastic group of chineses scientists, in the form of copper nanotubes or “CuNTs”.³ We prepared modified CuNTs with heterobiaryl endcaps. These caps contained either phenolate donors or cupric ions, to create male and female-type connections respectively. We anticipated that if similar connectors were incorporated into the other components of our computer, the CuNTs might self-assemble into complete circuits. A further benefit of CuNTs is their rigidity, which we hoped would prevent tangling.

Signal Output

The final component of our computer’s design was a means of expressing our PuPU’s output through the medium of visible

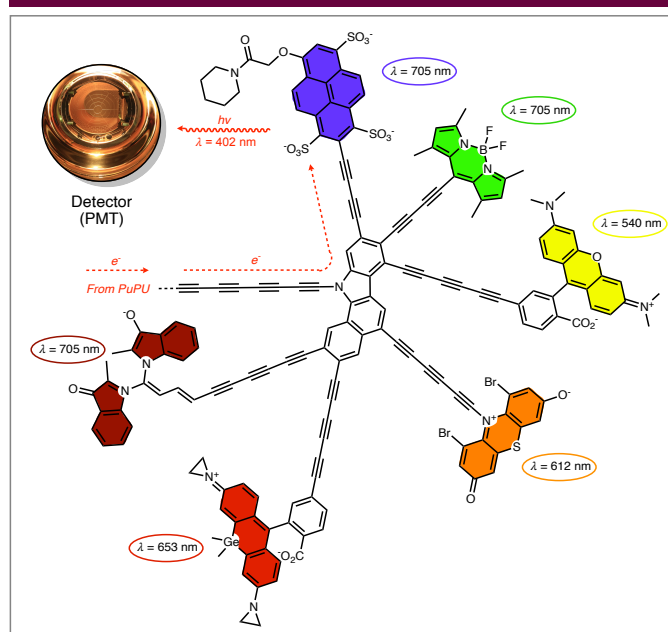


Figure 3: An example of a fluoroarray designed to serve as a molecular pixel, emitting a photon in one of six wavelengths when stimulated by an electron

light. To do this, we reverse-engineered the concept of our ChromeBoard™ by tethering a range of luminescent molecules to a conjugated scaffold. When stimulated by a PuPU-generated electron of the right energy, these fluorophores emit a photon in one of six frequencies between 400 and 700 nm. As such our device has twice the colour-depth of conventional RGB displays (Figure 3).

Unfortunately, we could only fit nine of these chromic arrays into our molecule. This meant that while the screen resolution was about 4.3×10^{14} pixels per square inch, the screen itself is only 20 micro-inches across. In practice, the in-game resolution is 3×3 pixels. Furthermore, our “screen” displays its information in batches of nine photons. This is considerably fewer than the $\sim 10^{18}$ photons per second emitted by a conventional computer screen.⁴ In fact, it’s so little light, we had to borrow some photomultiplier tubes (PMTs) from the Super Kamiokande neutrino detector in Japan.⁴ With the aid of these detectors, we were able to convert the DORF4000’s nine-photon output into a conventional video signal, which could be displayed on a standard monitor.

Assembly

With the individual components in hand, we used atomic force tweezers to position the PuPU, the ChromeBoard and the fluorophore arrays on a sheet of graphene. Next, the graphene was treated with a suspension of CuNTs (10^{-35} grains per cubic fathom). To our delight, SEM analysis of the graphene post-treatment indicated successful self-assembly of the CuNTs between the components of our device. Unfortunately, to acquire this SEM image, we had to coat the whole thing in gold, rendering it completely useless. Undeterred, we repeated the first two steps, and then used real-time Cryo-EM and a pair of nano-chopsticks to position our modified ribosomes and their tethered RNA polymerases adjacent to the PuPU. Finally, we transferred the hardware into a Tris-buffered solution of our DNA-encoded game data, contained within a $1 \mu\text{L}$ quartz Eppendorf tube. This mixture constituted our molecular computer.

While the DORF4000 is too small to be visible, the lasers, photomultiplier tubes, spectrometers and conventional computers required to operate it fill a medium-sized room. Furthermore, several technicians are required to operate it, making running costs quite high.

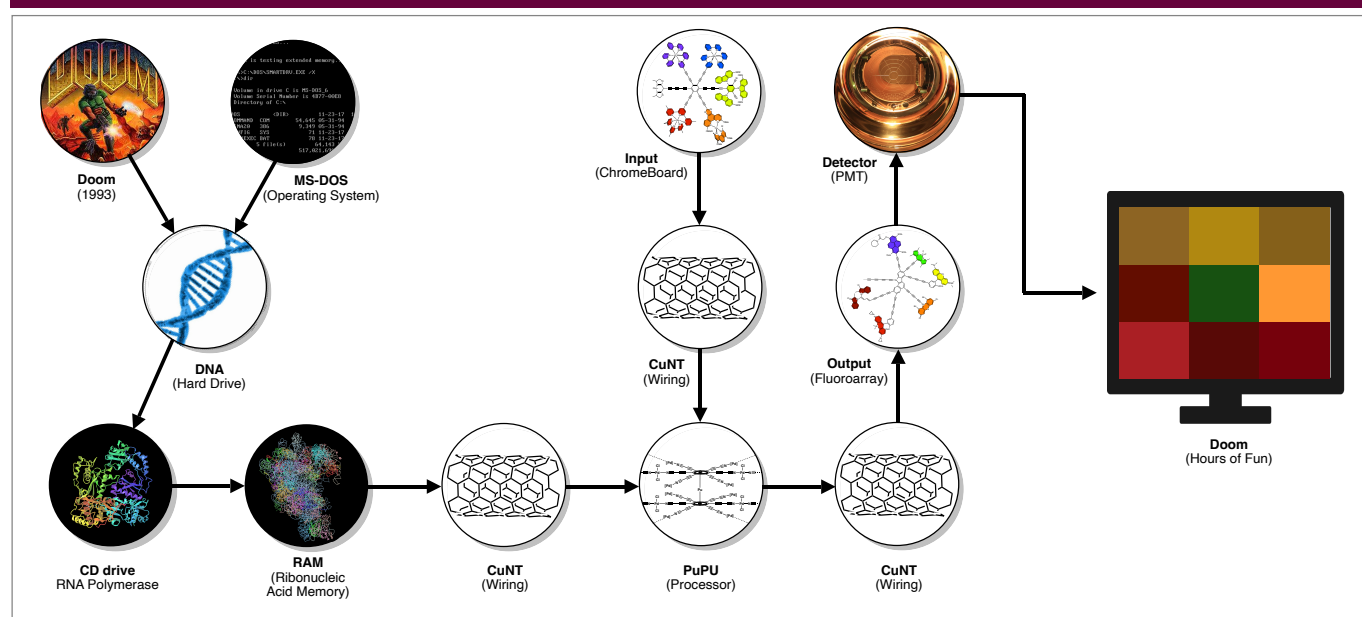


Figure 4: A schematic overview of the assembled DORF4000.

Operation and Gameplay

To boot up the DORF4000, transcription factors are added which correspond to the areas of the DNA encoding the operating system. When the levels of relevant mRNA have reached a suitable point (3-5 hours), further transcription factors are added to decode the game's data and opening screen. Once a new game has been started, Doomguy is controlled with the ChromeBoard™, which in turn is manipulated by shining one of five lasers on the Eppendorf tube. The scattered light from these lasers makes it quite challenging to detect the individual photons coming from our computer, as the signal to noise ratio is about 1:10¹⁴. We used an IBM Q1 supercomputer to execute real-time noise-cancellation calculations. As such, the lag-time between photons being emitted from the computer presented on-screen is only several minutes. This does make gameplay quite challenging, however. Figure 5 shows some comparisons of conventional Doom gameplay, and data acquired from our device.



Figure 5: Screenshots of doom running on an electric toothbrush (left) and on DORF4000 (right). Images on the right are composites extrapolated from the red, brown and grey photons emitted by DORF4000's fluoroarray.

If we're being entirely honest, we haven't made it out of the first room in "Knee Deep in the Dead" yet. This is partly because we can't find where we put the gene for setting difficulty level and it's stuck on "nightmare", but mostly because of the poor graphics and epic lag. However, that slight inconvenience should not detract from the fact that our molecular computer can run Doom (even if it can't run it well).

Conclusions

We have designed and fabricated the first functioning molecular computer, and demonstrated its capacity to perform the most basic of computational tasks: running Doom. Future work will focus on developing better graphics and incorporating HDMI compatibility, as well as fitting the rest of the keyboard in there somewhere.

Conflicts of Interest

Günther doesn't know anything about computer hardware, computer software, or molecular biology. Nor has he ever played Doom.

Notes and references

1. For examples of Doom running on ridiculous devices, see <https://www.reddit.com/r/itrundoom/top/?t=all>
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