Nanotechnology

Surface interaction propels molecule forwards

Leo Gross & Jascha Repp

The interaction of a molecule with a specific surface has been shown to produce consistent unidirectional motion driven by voltage pulses. The mechanism can even facilitate the transport of molecular cargo. **See p.82**

Living organisms are full of amazing molecular machines that have evolved to carry out many of the tasks that are crucial for life[1]. Artificial molecular motors are often smaller and, arguably, less complex than those found in nature, rendering them ideal models for understanding how natural motors work (see go.nature.com/3ry4kpn). On page 82, Simpson *et al.*[2] report a type of artificial motor that is smaller and simpler than most of those developed so far. And it's different, in that it's a molecular machine that gets along with help from the surface on which it moves – the molecule itself does not contain a motor unit. It's also extremely reliable, and can even push cargo, in the form of a single carbon monoxide molecule.

Scientists previously devised a molecular nanocar with four motor units[3], which could be driven forwards across a copper surface using voltage pulses applied with the tip of a scanning tunnelling microscope (STM). However, the molecule was relatively big and bulky, making it difficult to place it on the surface intact and image it. The team succeeded in showing that this single molecule could take around ten steps, but each step differed in size and direction from the previous one.

Another research group constructed a simpler motor that could rotate in one direction, using interplay between the molecule and the surface[4]. This aspect of the rotating motor is reminiscent of Simpson and colleagues' machine, but the latter moves across the surface in a linear manner. The reliability of this linear motor is remarkable – the authors' careful experiments showed that it could take 1,000 forward steps without a single step back.

The study also offers key insights into the motor mechanism on an atomic scale. A highly simplified analogy for the mechanism would be a type of railway trolley known as a handcar or draisine. This vehicle works by pumping a central 'see-saw' up and down to move it in one direction.

The parallels between a draisine and Simpson and co-workers' motor begin with the substrate. The molecule moves across a copper surface, and the crystal structure of this substrate provides a kind of train track (Fig. 1). On this track, the atoms are regularly spaced at intervals of 2.5 ångströms, defining the molecule's step length. There is a hydrogen atom at the centre of the molecule that can bind to either of two nitrogen atoms, resulting in two possible configurations. The molecule can be switched between these states to change its geometry and the way it binds to the substrate. The switching occurs with the help of electrons from the voltage pulse, applied by the STM tip[5], which provides the energy to run this motor. With the track and fuel determined, let's see how the draisine mechanism maps to these two molecular states.

The energy landscape associated with the site on the copper surface at which the molecule is adsorbed differs depending on the position of the central hydrogen atom. When the incoming electrons have sufficient energy (about 0.5 electronvolts), the molecule can switch from the low-energy to the high-energy configuration, and is driven out of its resting position (Fig. 1). The energy landscape of the high-energy configuration has a saw-tooth shape, so the molecule 'slides' down the saw tooth and moves in the forward direction. Finally, it returns spontaneously to the low-energy configuration and completes one step along the atomic lattice by moving to the next adsorption site.

Simpson *et al.* found support for this mechanism in a control experiment in which they replaced hydrogen with deuterium. Because deuterium has a larger mass than hydrogen, the voltage pulses that were required to move the deuterated molecules differed from those needed to propel the hydrogenated compounds. This indicates that switching of the hydrogen binding position (tautomerization) is involved in the process. In another control experiment, the authors increased the temperature from 7 kelvin to 40 kelvin – high enough to allow the molecules to move by thermal diffusion. As expected, the team observed that individual molecules moved forwards and backwards randomly along

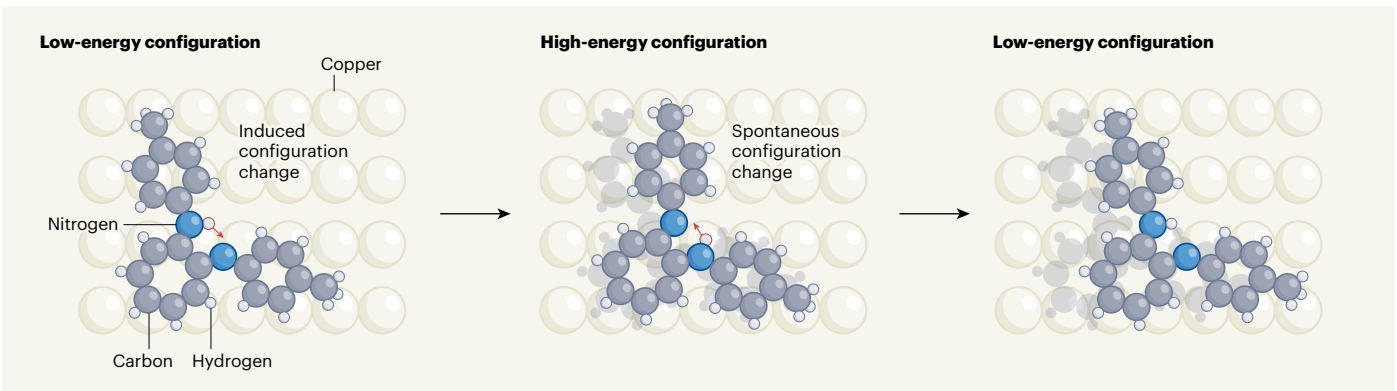


Figure 1 | A reliable artificial molecular motor. Simpson *et al.*[2] devised a molecular motor that moves across a 'track' on a copper surface (only the top layer of copper atoms is shown). A hydrogen atom at the centre of the molecule binds to either of two nitrogen atoms, and the application of a voltage pulse induces it to switch from one (low-energy configuration) to another (high-energy configuration). This change drives the molecule forwards along its track, after which it returns spontaneously to the low-energy configuration and completes the step. Simpson *et al.* showed that the molecule could take 1,000 forward steps without moving backwards once, and that it could push a carbon monoxide molecule across the surface.

the surface, in contrast to the unidirectional motion that was seen when movement was induced at 7 K.

The performance characteristics of such a tiny motor are hard to imagine; let's therefore compare this single molecule to a full-size car. The typical speed in the experiment, which was roughly one atomic step per second, is on the order of 10^{-9} kilometres per hour. And if the motor were pushing a carbon monoxide molecule over an energy barrier of 70 meV with each step, it would have a power output of about 10^{-23} kilowatts. It achieves this with fuel in the form of electrons from the tip of the microscope. To push its cargo, the experiments show that each step requires about 20 billion electrons, each with an energy of about 0.5 eV, which means that the motor consumes around 0.2 kilowatt-hours per 100 km. This is only one one-hundredth of the energy consumed by a real electric car, which can carry five people plus luggage.

One reason that the molecule consumes so much energy is that only one out of the 20 billion electrons that emerge from the tip of the microscope actually drives the molecule forwards by one atomic step, and all other electrons pass unused. This waste might be reduced in future implementations by simply increasing the voltage[5]. If such a motor could instead operate by changing its charge on an insulating surface, the electron yield might be on the order of one – that is, ten orders of magnitude higher than that of Simpson and colleagues' molecule – as shown previously for certain reactions[6] and molecular rotations[7]. Molecular motors can also be driven and controlled by light[8]. The versatility and functionality of the motors could be enhanced by selectively inducing chemical reactions[9].

Simpson *et al.* have presented a reliable and well-defined model system that surpasses the performance of other molecular motors.

"A highly simplified analogy for the mechanism would be a type of railway trolley known as a handcar or draisine."

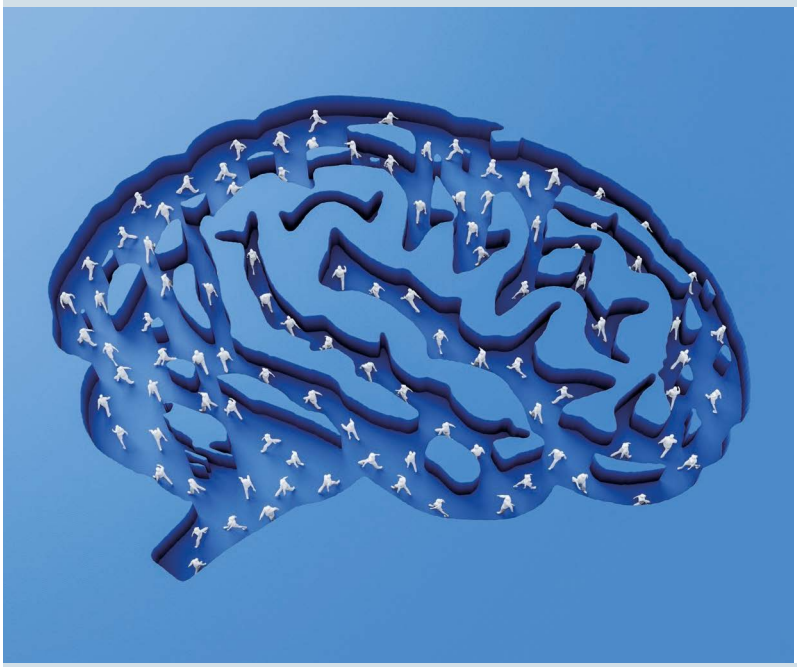
Such systems could be investigated in more detail to provide further insights into molecular machines; for example, atomic force microscopy could be used to enable resolution at the scale of atomic bonds[10]. Ultrafast STM set-ups[7] could even allow us to image these molecular motors in real time – another truly fascinating goal.

Leo Gross is at IBM Research Europe – Zurich, 8803 Rüschlikon, Switzerland. **Jascha Repp** is in the Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany.
e-mails: lgr@zurich.ibm.com; jascha.repp@physik.uni-regensburg.de

1. Erbas-Cakmak, S. *et al. Chem. Rev.* **115**, 10081–10206 (2015).
2. Simpson, G. J., Persson, M. & Grill, L. *Nature* **621**, 82–86 (2023).
3. Kudernac, T. *et al. Nature* **479**, 208–211 (2011).
4. Stolz, S., Gröning, O., Prinz, J., Brune, H. & Widmer, R. *Proc. Natl Acad. Sci. USA* **117**, 14838–14842 (2020).
5. Liljeroth, P., Repp, J. & Meyer, G. *Science* **317**, 1203–1206 (2007).
6. Fatayer, S. *et al. Phys. Rev. Lett.* **121**, 226101 (2018).
7. Peller, D. *et al. Nature* **585**, 58–62 (2020).
8. Saywell, A. *et al. ACS Nano* **10**, 10945–10952 (2016).
9. Albrecht, F. *et al. Science* **377**, 298–301 (2022).
10. Gross, L., Mohn, F., Moll, N., Liljeroth, P. & Meyer, G. *Science* **325**, 1110–1114 (2009).

The authors declare no competing interests.

scientific reports



Publish your research in psychology

You will now find a brand-new section of *Scientific Reports* content dedicated specifically to psychology, with the aim of addressing the psychology community's specific needs.

- **Expert** Editorial Board to manage your paper
- Follows Nature Portfolio's **high peer review standards**
- Indexed in **Web of Science, PubMed** and other major repositories
- Research accessed from over **180 countries worldwide**

nature.com/srep

nature portfolio