

## Maths, Physics &amp; Chem

## How an artificial molecular machine pumps in nanoscale

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*Chemists tend to take inspiration for innovation from nature. A team led by the Nobel Prize winner J. Fraser Stoddart developed a fully artificial molecular pump, which works in a similar way to biomolecules. Achieving precise control of the pump's motion – driven by electricity and light – opens the door to designing more complex molecular machines.*



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Nature often uses sophisticated strategies beyond our imagination. For example, biomolecules such as enzymes and nucleic acids form dynamic networks, in which they loosely associate with each other only when they need to perform a task together. Taking inspiration from such weak and temporary interactions, along with advanced technologies, scientists have recently invented artificial molecular machines. Movements of these synthetic molecules – driven by loose interactions – can be controlled to carry out tasks at the nanoscale. Such molecular machines have great potential for many different applications, such as creating artificial cells or light-harvesting systems. The 2016 Nobel Prize in Chemistry was awarded to Sauvage, Feringa and Stoddart for their work in that field.

In a new study, the researchers set out to achieve a more precise control of the machine's motion, and introduced a so-called 'molecular pump'. It is based on an artificial molecular architecture named rotaxane – consisting of two separable parts: a dumbbell-shaped part and a ring-shaped part. It works like a classic hand pump – which mechanically carries water (the ring) up from the underground (the environment) by hands (external power).

What's innovative about this machine is that the association of the ring with the dumbbell can be controlled. In other words, the ring can be either free from the dumbbell ('on') or be trapped around the dumbbell shaft ('off') by the two bulky ends. As an additional small molecule can be attached to the ring, we could employ the ring as a carrier that, for

example, delivers a drug to a specific place in the body. In this case, the drug remains inactive when trapped on the dumbbell shaft but can react with its target once it is released from it, allowing us to control the timing of drug delivery.

This new molecular pump runs as an 'on-off-on' system. This means that the operation has two steps – the recruitment of the ring (on-to-off) and its release into the environment (off-to-on) – which we can control using electricity and light (external powers). The first step is the recruitment of the ring from the solution (the environment) and it's controlled by electricity. By fine-tuning the electrical energy, the ring is first recruited, then strongly pushed to pass over the bulky end of the dumbbell called 'speedbump' to reach the inside of the pump's architecture. These events resemble how a classic hand pump operates – lifting the piston to bring the water up (recruiting the ring), then pushing the piston down pushes the water through the outlet (pushing the ring over the speedbump) so that we can harvest water.

Unlike the classic pump, the ring doesn't come out through the outlet yet, as the outlet is closed by the other bulky end of the dumbbell, called the 'stopper'. In other words, the recruited ring is now trapped within the architecture and can freely move between the two bulky ends: the speedbump and the stopper. The release of the ring is driven by light – the stopper breaks down when irradiated with UV light. When the stopper is removed, the ring is released to the solution, where it and its possible appendage (e.g. drug) can freely react on the target.

In summary, the researchers created the artificial molecular pump that can deliver its small separable part (the ring) carrying a possible useful molecule. The pump's two-step operation – the ring's recruitment (by electricity) and its release (by light) – allows precise control of its motion in time and space. Although this work is more knowledge-oriented than application-oriented, the controllable delivery of the ring that can carry an additional cargo could prove useful, for instance for drug delivery. The beauty underlying fundamental research is that it creates seemingly purposeless tools, which might then find an application in another field of research.