CHEMISTRY

Nanoscale Bulldozer

Scientists discover a one-molecule motor that hops in straight lines

IN A BASEMENT room at Austria's University of Graz sits a jumble of steel tanks and ice-encrusted tubes. The contraption, a scanning tunneling microscope, can snap pictures of individual atoms and molecules. It's so sensitive that it works best at night, when nobody's around to walk or talk or otherwise rattle the building.

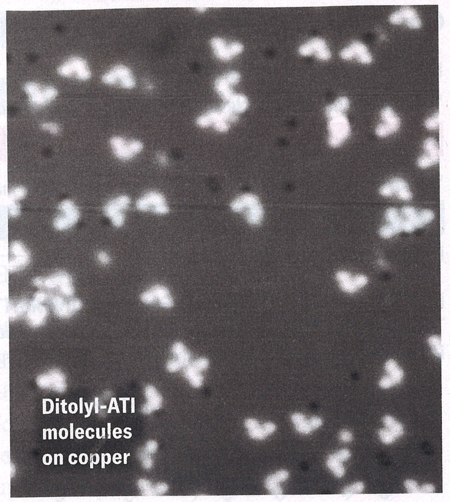
A computer monitor beside the machine shows images of tiny, heart-shaped blobs arrayed over a copper surface. The "hearts" are individual molecules: ditolyl-ATI molecules, to be precise. Earlier this year Grant Simpson, a chemist in the microscopy laboratory, had been playing around with them, hoping they could be coaxed to act like minuscule mechanical switches.

What he found instead was far more intriguing. When excited with an electrified microscope tip, the molecules jumped—but they didn't hop around willy-nilly. "Somehow," Simpson says, "I'd come to the realization, slowly, that they're only moving in one direction."

The hopping hearts are an entirely new kind of molecular nanomotor—a tiny machine that expends energy to move purposefully against the entropic tides that constantly pull the small-scale world into random, useless motion. Some human-made nanomotors can spin in place, but few can reliably move from point A to point B. The mechanical magic of the new motor, described recently in *Nature,* comes from the interaction between the molecule and the copper surface it moves along—as if a train engine had parts both in the car and embedded in the track below.

It's a small but significant step toward the dream of a nanotechnology that can build things nature's way: bottom-up, atom by atom. "If we build a chair, we take a tree, and we cut it down," says physicist Leonhard Grill, Simpson's colleague at the University of Graz. "Nature does it the opposite way. Nature grows the tree." Researchers developing miniature machines imagine using them to create novel materials, to supercharge industrial catalysis and to manipulate biological tissues with the agility of real enzymes.

"Miniaturization has always driven advances in technology," says chemist David Leigh of the University of Manchester. But the problem with nanotechnology, he explains, is that the familiar mechanics of the "big world" simply don't work on the molecular level. At such tiny scales, randomness rules. If properties such as temperature, energy and pressure are held steady, then small-scale processes—including chemical reactions or the movements of particles—are equally likely to happen in every direction. Moving from A to B at the nanoscale is like rolling a die and taking steps forward, backward or sideways depending on the result. "You can't use Newtonian mechanics" in nanotechnology, Leigh says. "That basically rules out all the engineering processes that we've built up as civilizations over the past 5,000 years."



Ditolyl-ATI molecules on copper

From "Adsorbate Motors for Unidirectional Translation and Transport," by Grant J. Simpson et al., in *Nature,* Vol. 621; September 6, 2023

So why do scientists think it should be possible to develop nanoscale machinery at all? Leigh says the answer is that there's already a mature and working example out there, "and it's called biology." The intricate natural enzymes that flap a bacterium's flagella, twitch an animal's muscles and synthesize chemical energy in a cell's mitochondria are all molecular machines.

In 1999 scientists synthesized the first true molecular nanomotor, a light-powered rotary motor that was later recognized with a Nobel Prize in Chemistry. Since then, scientists have developed many more types of motors with different capabilities. University of Groningen chemist Nathalie Katsonis and her colleagues recently stuck trillions of nanorotors together and synced them up to physically move a macroscopic polymer. And Leigh and his colleagues have developed rotary nanomotors that, like biological enzymes, move by harnessing energy from chemical reactions catalyzed by the motor itself.

But rotary motors spin in place; molecular motors that move in straight lines, like trains on tracks, have proved a greater challenge to build. Some researchers have synthesized ring-shaped molecules that can rotate and slide along dumbbell-shaped scaffolds. Then there are DNA "walkers," which have legs and move by taking steps, like some biological motor proteins. But DNA walkers are relatively hefty (not strictly "nano," Leigh says) and can take only a handful of strides along carefully prefabricated nucleic acid tracks. The new heart-shaped motor, though, is just a few nanometers across and will keep hopping along its track of copper atoms as long as the surface isn't interrupted.

Simpson and Grill discovered the motor mostly by accident—it was "pure serendipity," Grill says. The scientists were initially intrigued by how the ditolyl-ATI molecule tosses one of its hydrogen atoms back and forth between its two nitrogen atoms, a behavior the scientists thought could make it useful as a nanoscale switch. After years of work, Simpson tried depositing the molecules on a particular kind of copper surface in which the atoms are arranged in linear rows. To his surprise, a jolt of electricity sent the hearts hopping along the copper tracks. The researchers then confirmed that the molecules move in just one direction and can even push along other particles like nanoscale bulldozers.

This new motor is an "energy ratchet," says Katsonis, who was not involved in the study. It uses energy—here a jolt of electricity—to switch between two states, each with a different set of energetic possibilities. Zapping the molecule makes it lurch into its more excited state, in which moving forward along the copper rail is favorable. When the molecule falls back down to its original, unexcited state, it jumps exactly one step forward along the track.

"In my opinion, it's interesting for two reasons," Katsonis says. First, the molecules interface with something bigger than themselves, in this case a surface. Second, they move in a line along an atomic track—the key to mastering directional motion at the nanoscale, she says. After all, biology's many linear molecular motors typically strut along scaffolds to travel in the right direction.

"This is really nice because it's just moving one-dimensionally, directionally, in a very minimalist system," Leigh says. The new energy ratchet probably won't propel a nanobot or assemble a tree atom by atom anytime soon. But it can be easily studied with scanning tunneling microscopes, making it a perfect test system for future experiments with energy ratchets, tracks and directional motion—and Katsonis and Leigh say that's a big hop in the right direction.

—Elise Cutts

Mine Spotting

An AI model could help clear land mines

AI Finding and removing land mines is an excruciatingly slow process. Human deminers scour contaminated ground inch by inch with handheld metal detectors, waiting for the telltale beep of a magnetic anomaly. Although trained dogs are sometimes used, metal detectors have remained the go-to clearance method since the end of World War II.

"There's a very long period where there hasn't been much innovation in the field," says Jasper Baur, a Ph.D. student in volcanology and remote sensing at Columbia University. Baur and his collaborators at Safe Pro Group, a manufacturer of personal protective gear, have been developing a drone-based machine-learning technology to make demining safer and faster than with traditional methods.

The idea is deceptively simple: A drone flies over an area thought to be mined, collecting a large volume of images. Baur's algorithm, trained on the visual characteristics of 70 types of land mines, cluster munitions, and other unexploded ordnance, processes the images into a map, with resolution down to a fraction of an inch. The model can then recognize and map explosives more quickly and accurately than a human reviewing the same images. "In a matter of minutes you'll have a map plotted out with where all the land-mine detections are," Baur says.

With a reported detection rate of about 90 percent, the drones are meant to augment traditional methods, not replace them. "It's less comprehensive because you're not going through inch by inch," Baur says. But the approach can reveal potential dangers and can cover more ground than manual efforts.

Baur and his team have visited Ukraine to test the technology multiple times since the start of the war there. They hope their work can speed up a demining process that, using current resources, could take more than 750 years. By some estimates, Ukraine has about 67,000 square miles (an area roughly the size of Florida) that could harbor mines and other explosives. With the new system, "you can scan wide areas of land and try to figure out where the highest density of contamination is" before sending in humans to defuse the mines, Baur says.

For now the AI can detect only surface-level explosives, not deeply buried ones or those covered by vegetation. Baur's nonprofit organization, the Demining Research Community, is testing ways to look deeper by using thermal imaging and ground-penetrating radar. It is also developing a model that can rate the AI's level of confidence in its mine-detection results based on the amount of vegetation present.

Milan Bajić, an expert in remote sensing who has been involved in demining efforts in Croatia, says the approach is a valuable addition to the demining tool kit. "There is no silver bullet of technology," he says, "but combining different technologies can be more successful than any of them."

—Lori Youmshajekian