

Progress through Mechanics: *Artificial Molecular Machines*

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Human bodies have many molecular motors and machines [1]. In these biomotors, nature demonstrates most elegantly that simple molecular mechanical components, once organized and assembled in a precise manner, can link motions efficiently from the nanometer scale to the macroscopic world, and achieve complex functions such as powering skeletal muscles, synthesizing ATP (the energy source for most living creatures), and producing DNA/RNA (the origin of life). For example, the contraction and extension of natural muscles, the “best of the best” among the existing actuators, takes place by mutual sliding between myosin fibers (polymer of biomotors) and actin filaments. When appropriately oriented and organized, collections of these myosin/actin nanocomposite materials can give rise to substantial macroscopic movements in human muscle.

Compared to biomotors, artificial molecular machines have a much shorter history. In 1959, Richard Feynman, one of the greatest physicists of the twentieth century, originated the idea of artificial molecular machines in his historic address “There is Plenty of Room at the Bottom [2].” The Nobel laureate contemplated, “*What are the possibilities of constructing molecular-scale mechanical machines ... What would be the utility of such machines? Who knows? I cannot see exactly what would happen, but I can hardly doubt that when we have some control of the arrangement of things on a molecular scale we will get an enormously greater range of possible properties that substances can have, and of the different things we can do.*” In the past two decades, employing the concepts of self-assembly and molecular recognition, chemists have successfully synthesized artificial molecular machines such as bistable rotaxanes [3, 4]. Upon the application of an external stimulus (electricity, light, or chemical reagent), the ring component of a bistable rotaxane molecule can be switched back and forth between the two recognition sites along a dumbbell-shaped component, thereby enabling the molecule to behave like a linear molecular motor.

Such molecular motors with controllable mechanical motions are integral components in developing functional nanosystems for nanotechnology. For example, as actuation materials, bistable rotaxanes have at least six advantages: (1) They can generate large strains up to 42%, while the strains generated by the gold-standard actuation materials – piezoelectric materials – are typically 0.1–0.2% [5, 6]. (2) They have a high force density, e.g., a bistable rotaxane can generate ~100 pN force, while a kinesin biomotor, which is much larger than a bistable rotaxane, can only generate 6 pN. (3) They can undergo controlled mechanical motion for a variety of external stimuli, while traditional actuation materials and biomotors must both rely on a single stimulus. (4) They can be customized and optimized, therefore conferring the flexibility necessary for a multitude of engineering applications. (5) They can survive in a wide range of temperatures (-30 –100°C) and pH values (4–10), while biomotors are restricted to physiological conditions ($T \sim 37^\circ\text{C}$, $\text{pH} \sim 7$). This characteristic indicates that although *biomotors* are perfect

actuators in human bodies, *artificial* molecular machines such as bistable rotaxanes are more suitable “molecular actuators” for human-made devices.

Inspired by artificial molecular machines’ tremendous potential as actuation materials, several research groups have been aiming at developing mechanical systems that operate with the same elegance, efficiency, and complexity as biological motors function within the human body. Although this is still a lofty goal today, some impressive progress has been made in this exciting research direction in recent years. Different groups have proven that once organized, various forms of nanomachines (<10 nm) can be used to manipulate much bigger objects (e.g., microcantilever beams, submillimeter-sized glass rods, and microliter droplets), mimicking what biomotors have achieved in human muscles:

Bending microcantilever beams: Huang and colleagues have created a cantilever actuator powered by rotaxane “molecular muscles” [7]. The rotaxane was comprised of a symmetric dumbbell component with two rings interlocked onto the dumbbell. The distance between two rings contracted upon oxidation of the rotaxane, while it extended upon reduction. Each ring carried a disulfide tether which allowed the rotaxane to self-assemble on a gold surface by means of its two rings. These “molecular muscles”, when self-assembled on microcantilever beams (500×100×1 μm), were capable of bending and stretching the beams when appropriate redox reagents were injected into the device environment. Using elementary beam theory and analysis, it was shown that these observations support the idea that cumulative nanoscale movements within surface-bound “molecular muscles” can be harnessed to perform larger-scale mechanical work.

Rotating submillimeter-sized glass rods: Another illustration of the power of molecular machines was completed by Eelkema and colleagues [8]. They fabricated light-driven, unidirectional molecular rotary motors embedded in a liquid-crystal film; these motors were capable of rotating a glass rod that was roughly 10,000 times larger than the motors. The motor was comprised of a rotary part (a right-handed helical structure), an axle (a central carbon–carbon double bond) and a stator part. Upon doping a non-polymeric liquid-crystal (LC) film with the motors, the helical organization induced by the motors resulted in a polygonal fingerprint texture in the surface of the film. The rotation of the texture in the motor-doped LC film was used to manipulate a glass rod (5 μm by 28 μm) placed on top of the surface.

Transporting microliter droplets: Berna and his colleagues demonstrated the use of a molecular machine-based photoresponsive surface to control macroscopic liquid transport across surfaces [9]. When small drops of low-volatility liquids (e.g., CH₂I₂) were deposited onto the photoresponsive surface, the collective operation of the rotaxane monolayer was sufficient to power the movement of a 1 μL droplet up a 12° incline. In this experiment, roughly 50% efficiency was achieved; approximately half of the light energy absorbed by the rotaxanes was used to overcome gravity.

By harnessing the nanoscale mechanical motion from artificial molecular machines to elicit a mechanical response in larger-scale systems, the described designs mimic natural skeletal muscles. Although challenges remain, we believe that with collaboration from experts in multiple disciplines (such as mechanics, chemistry, physics, and mathematics), the

comprehensive design, construction, and application of molecular machine-based nanomechanical systems will become possible.

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