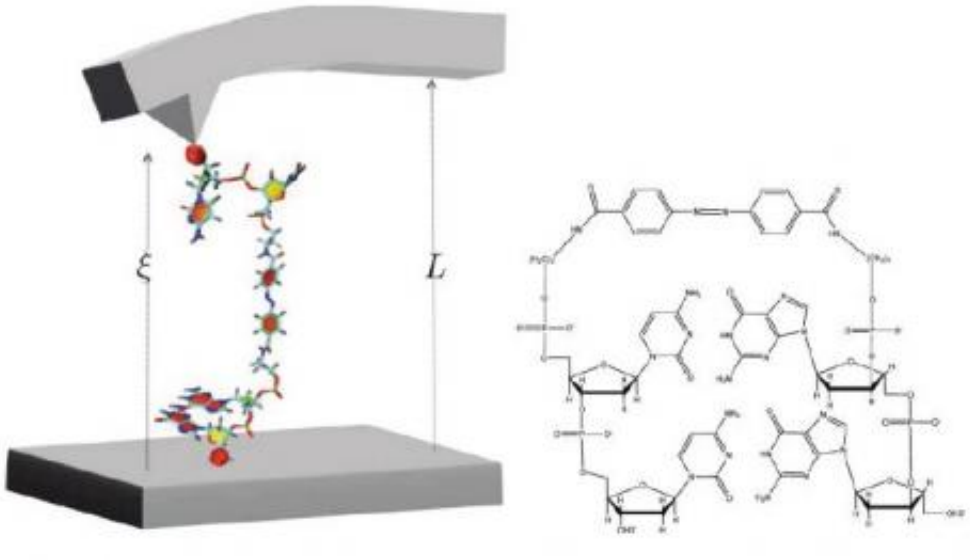
Researchers turn photons into work using DNA

March 10 2011, By Lisa Zyga



(Left) An illustration of the DNA-based molecular motor. The molecule is extended in its soft cis mode, and then contracted back to its original size in its stiffer trans mode, when work is extracted. (Right) An illustration of the DNA's structure. Image credit: McCullagh, et al. ©2011 American Chemical Society.

(PhysOrg.com) -- By using light to change the elasticity of a DNA molecule, scientists have designed a molecular motor that can turn light into mechanical work. Unlike most previously reported molecular motors, the proposed setup involves an atomic force microscope, which acts as an interface with the outside world and enables the work to be extracted.

The researchers, Martin McCullagh, Ignacio Franco, Mark A. Ratner, and George C. Schatz, from the Department of Chemistry and the Non-equilibrium Energy Research Center (NERC) at Northwestern University, have published their study in a recent issue of the Journal of the American Chemical Society.

The molecule that the scientists propose using as the central component of the motor is a DNA hairpin that includes two guanine-cytosine base pairs capped by an azobenzene compound. The scientists designed a computational model of the system including the attachment of one end of the DNA hairpin to a surface and the other end to an atomic force microscope coupled to a cantilever.

“The greatest significance of this work is showing how the structure of DNA can be exploited to amplify the transduction ability of azobenzene in a setup in which the work can be extracted,” Schatz told *PhysOrg.com*. “To our knowledge, this is the first proposed DNA-based molecular motor with an interface to the outside world.”

In their molecular dynamics simulations, the researchers used light to change the structure of the azobenzene. In this process, called “isomerization,” the DNA-motor reversibly changes between the cis isomer and the trans isomer. Although this photoinduced isomerization is only a structural change, it has important implications, such as changing the length of the molecule (the trans isomer is longer) and altering the stability of the bonds between the guanine and cytosine bases (the trans isomer’s intra base pair interactions are stable across a greater range of lengths).

As the chemists showed, these two differences between the cis and trans isomers alter the molecule’s elasticity, and can be exploited to extract work from the system. For modest extensions, the trans isomer of the DNA hairpin is stiffer because it has a geometry that favors DNA base

pairing, which makes it more difficult to extend the DNA hairpin.

To extract work from the system, the scientists proposed using a single-molecule analog of a thermodynamic cycle (a Stirling cycle). In this cycle, the molecule in its soft cis mode is first extended using the AFM setup. Next, light transforms the cis isomer into the stiffer trans isomer. The trans structure is then contracted to the motor's original extension. Finally, a second light source is used to isomerize the molecule back to the cis state to close the cycle. Since the molecule is stiffer during contraction, the work extracted during contraction is larger than the work invested during extension, leading to net work extraction.

"The basis of this motor is the photoinduced change in elasticity of the azobenzene-DNA molecule," Schatz said. "Because of the setup, the AFM is an integral part of the DNA motor. Work must be done on the molecule and cantilever to extend it, and work is extracted from the composite system during contraction. If the molecule is stiffer during contraction, then net work can be extracted."

The scientists estimated a maximum of 3.4 kcal/mol of extractable work per cycle with an estimated maximum efficiency of 2.4%. This amount of work is comparable to the 7.3 kcal/mol of free energy output in ATP hydrolysis, which is the main energy source in biological processes.

"While the amount of extractable work from this motor is promising, the focus of this study is on investigating novel concepts in energy conversion," Schatz said. "The proposed DNA-based motor provides a platform upon which further improvements can be made. We would like to highlight that the explored setup provides a means to quantify the transduction abilities of single molecules. Such quantification is a pivotal step in transforming single-molecule machines from scientific curiosity to actual power supplies for nanoscale processes."

In the future, the scientists plan to use these insights regarding the relationship between a molecule's structure and its function to improve the DNA-based motor design. They hope to find more optimal azobenzene-capped structures, as well as investigate the effect of temperature on the motor's performance.

More information: Martin McCullagh, et al. "DNA-Based Optomechanical Molecular Motor." *Journal of the American Chemical Society*. DOI:10.1021/ja109071a

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Citation: Researchers turn photons into work using DNA (2011, March 10) retrieved 28 April 2024 from https://phys.org/news/2011-03-photons-dna.html

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