Molecular Machines—Rotors and Shuttles

Chen Zhang Literature Seminar November 14, 2002

Following Nobel Laureate Richard Feynman's pioneering talk "There's Plenty of Room at the Bottom" in 1959[1], scientists begin to explore the fascinating, yet formidable field of molecular machines. With the development of lithography technology driven by the insatiable appetite of the semiconductor industry, a "top-down" approach to molecular machines has been pursued by a lot of physicists and engineers. This approach is to try to miniaturize existing macroscale machines to micro- or even nano-scale. Alternatively, a "bottom-up" approach, which aims at developing new motion systems on single-molecular level without much similarity to macroscale counterparts, seems more promising. Chemists, already at the "bottom"—manipulating atoms and molecules, are therefore ideal for exploring the "bottom-up" approach.

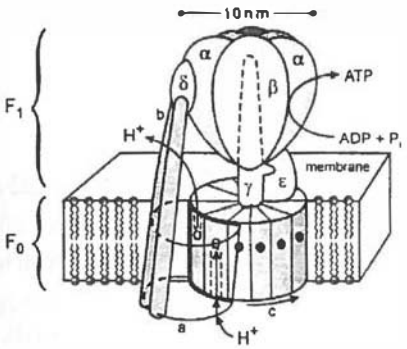

Figure 2

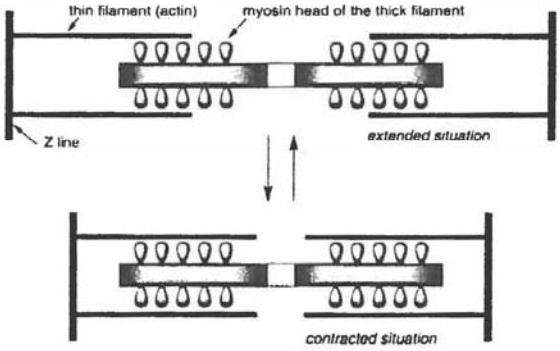

Figure 3

Similar to all the other fields in science, human beings have always been asking nature for the first step. There are a variety of molecular machines existing in biological systems, developed by the powerful evolution.[2,3] Two of the most studied cases are probably ATPase (**Fig. 1**) as a biomolecular rotor[4], and myosin (**Fig. 2**) as a linear motor[5,6]. Single molecular machines based on biomolecules such as DNA[7] have been made.

Molecular machines are defined as "an assembly of a distinct number of molecular components that are designed to perform machinelike movements (output) as a result of an appropriate external stimulation (input)".[8] The main building blocks are interlocked macromolecules—[2]rotaxanes and [2]catenanes.[9] [2]Rotaxanes represent a group of compounds with a dumbbell-shaped molecule encircled in a macrocycle, while [2]catenanes are compounds with two mechanically linked macrocycles.

A huge variety of molecular machines capable of doing different movements have been made in the past decade, including molecular turnstiles[10], gears[11], rotors[12-15], shuttles[16-19], plugs[20,21], and switches[22,23]. Among those applications, molecular rotors

(**Fig. 3**) and shuttles (**Fig. 4**), mimicking ATPase's rotational motion and myosin's linear motions, are most challenging due to the complexity of their motions.

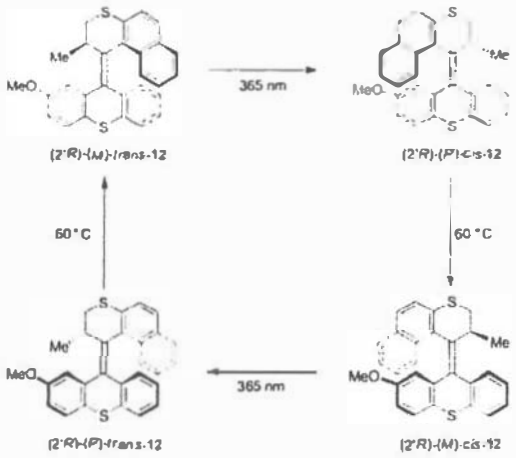

Figure 4

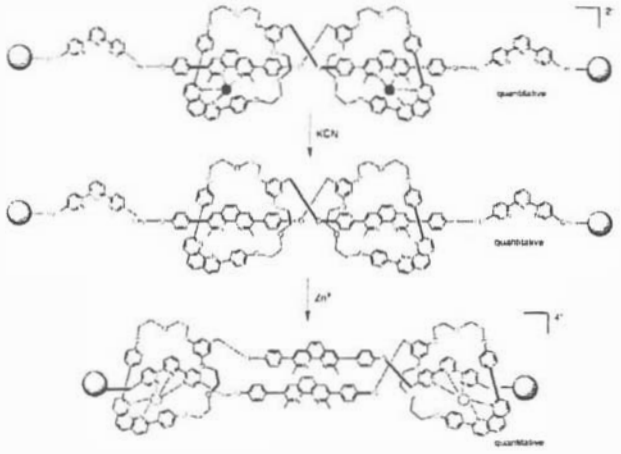

Figure 5

Virtually, all organic molecules containing a C-C single bond can be considered a molecular rotor, performing the rapid Brownian rotation. But those rotations are generally useless in term of doing mechanic work, due to the lack of control. Steric hindrance[10] can be employed to eliminate the freedom of motions, thus allowing more control over the rotation. Stronger control can be achieved using H-bonding[14]. Recently, two groups succeeded in assembling unidirectional rotors driven by chemical reaction[13] and light[12], respectively. Color tuning of liquid crystal by controlled rotation of a single molecular rotor is accomplished recently.[24]

Molecular shuttles are mostly based on [2]rotaxanes, due to their natural linear molecule—'track' and movable macrocycle— 'shuttle' structure.[8] Movement of the 'shuttle' along the 'track' is realized by the recognition mechanisms of the 'stations', recognition sites on the linear molecular. The linear motion can be triggered by means of outside stimulus and controlled by tuning the affinity of the 'shuttle' to the 'stations'. The stimulus—'fuel' for the shuttle can normally be either electrochemical[16], photochemical[18] or chemical[16,17]. Further advances have been made on mimicking the stretching movements of muscles[19] using similar ideas as molecular shuttles.

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