Title of Project：Development of supramolecular tools for control of chemical events

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Research Area：Chemistry

Keyword：Supramolecule, Molecular Devices, Functional Catalysts

【Purpose and Background of the Research】

The objective of the research is to develop novel supramolecular tools that are able to control chemical events such as “chemical reaction” and “energy conversion” by mimicking the functions of biological molecules.

Stimuli responsive molecules have been attracting attention as key components of molecular devices such as molecular sensors and memories. We have focused our attention on “molecular machines” that undergo mechanical motions in response to stimuli, and designed conceptually new molecules that realize elaborate programmed motions. On the other hand, the recent progresses in molecular biology have shown us that many biological events occur with mechanical motions of biological molecules. These new findings have shown the new directions for possible application of synthetic molecules. The objective of the research is to control “chemical reactions” and “energy conversion” by synthetic molecular machines.

【Research Methods】

The key concept of the research is “reversible switching of the mechanical distorsion of molecules”. It is well known that the steric environment around the reaction center affects on the activity of synthetic catalysts or enzymes. If the distortion of such catalytic molecules could be controlled by molecular machines through their mechanical motions, one can reversibly switch the reactivity as desired. This principle is simple, and would be applicable for various chemical events. Furthermore, the molecules would store energies through mechanical distortion, which could be converted into another type of chemical energy. The first objective of the research is to develop molecular machines, which interact with organometallic catalysts and enzymes through intermolecular interactions, and control their activities through mechanical motions. The second objective of the research is to develop molecular machines beyond molecular switches. In the case of molecular machines which undergo reversible motions between two states, it is essentially difficult to extract real “works” from these motions. On the other hand, biological systems realize the multimodal motions by making use of the ATP hydrolysis process including ATP binding, hydrolysis of ATP, and release of resulting ADP. Such multimodal processes realize, for example, directional transportation of substances as was found in the kinesin/microtubule system. By using synthetic catalytic systems, it would be able to realize multimodal motions like biological molecular machines.

【Expected Research Achievements and Scientific Significance】

The chemical events occurring in biological systems, including molecular machines, are highly effective in terms of energy efficiency. Development of synthetic molecular tools, targeting the control of chemical events by mechanical motions, would possibly show new directions for functional molecules.

【Publications Relevant to the Project】

Mechanical Twisting of a Guest by a Photoresponsive Host, Takahiro Muraoka, Kazushi Kinbara, and Takuzo Aida, *Nature* **2006**, *440*, 512–515.

Chaperonin-Mediated Stabilization and ATP-Triggered Release of Semiconductor Nanoparticles, Daisuke Ishii, Kazushi Kinbara, Yasuhiro Ishida, Noriyuki Ishii, Mina Okochi, Masafumi Yohda, and Takuzo Aida, *Nature* **2003**, *423*, 628–632.

【Term of Project】 FY2009-2013

【Budget Allocation】 69,400 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.tagen.tohoku.ac.jp/labo/kinbara/index.html