【Grant-in-Aid for Scientific Research (S)】

Biological Sciences (Medicine, Dentistry, and Pharmacy)

Title Project : New Molecular Technologies to Open Up Multiple Applications of Light in Life Science and Materials Science

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Research Project Number : 17H06173 Researcher Number : 00271916
Research Area : Organic Synthesis, Elements Chemistry, Theoretical Chemistry
Keyword : Molecular Transformation, Material Science, Spectroscopy

【Purpose and Background of the Research】

Complex π-electron compounds that interact with light have long attracted interest, and have become increasingly important in recent years for potential applications in life science and materials science. However, there are still severe limitations in rational design, synthesis, and derivatization of π-electron organic molecules, as well as in their functional modification (absorption/emission properties, quantum yield, thermo-stability, *etc.*), and these issues have hampered their practical application in advanced technologies, including storage media, organic semiconductors, laser printers, photodynamic therapy of cancer, nonlinear optics, deodorants, and molecular imaging. This project aims to develop new synthetic methods, to extend theoretical principles, and to synthesize novel π-electron molecules with unique functionalities suitable for next-generation technological applications.

【Research Methods】

Interdisciplinary research from various viewpoints, including organic chemistry, physical chemistry, and theoretical chemistry, is needed to develop novel functionalized π-electron molecules for many future applications. We intend to focus on the following four areas:

① Breakthrough synthetic chemistry to construct π-electron molecules and to provide new tools for chemo-, regio- and stereo-selective introduction of various functional groups into π-electron molecules
② Molecular science for the utilization of light
③ Theoretical chemistry to underpin the utilization of light
④ Molecular technology for the utilization of light

【Expected Research Achievements and Scientific Significance】

Besides providing new molecules, tools, and theoretical principles, one of the specific aims of this project is to create near-infrared light-capturing π-electron compounds. Such compounds could be useful for cancer treatment by photodynamic therapy, *in-vivo* 3D imaging, and many other purposes. As near-infrared light penetrates well through human tissue, compounds that absorb strongly in this wavelength region are particularly desirable for photodynamic therapy, since specific illumination of the tumor would allow only cancerous cells to be heated/damaged and consequently killed.

【Publications Relevant to the Project】

・N. Toriumi, A. Muranaka, E. Kayahara, S. Yamago, M. Uchiyama "In-plane Aromaticity in Cycloparaphenylene Dications: A Magnetic Circular Dichroism and Theoretical Study" *J. Am. Chem. Soc.,* **137**, 82-85 (2015)
・D.-Y. Wang, M. Kawahata, Z.-K. Yang, K. Miyamoto, K. Yamaguchi, C. Wang, M. Uchiyama, "Stille Coupling *via* C–N Bond Cleavage" *Nature. Commun.*, **7**, 12937 (2016)
・N. Tezuka, K. Shimojo, K. Hirano, C. Wang, T. Saito, R. Takita, M. Uchiyama, "Direct Hydroxylation and Amination of Arenes via Deprotonative Cupration" *J. Am. Chem. Soc.*, **138**, 9166–9171 (2016)
・M. Tanioka, S. Kamino, A. Muranaka, Y. Ooyama, H. Ota, Y. Shirasaki, J. Horigome, M. Ueda, M. Uchiyama, D. Sawada, S. Enomoto, "Reversible Near-Infrared/Blue Mechano-fluorochromism of Aminobenzopyranoxanthene" *J. Am. Chem. Soc.,* **137**, 6436-6439 (2015)

【Term of Project】 FY2017-2021

【Budget Allocation】 163,300 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.f.u-tokyo.ac.jp/~kisoyuki/