【Grant-in-Aid for Scientific Research on Innovative Areas (Research in a proposed research area)】
Science and Engineering

Title of Project : π-System Figuration: Control of Electron and Structural Dynamism for Innovative Functions

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【Purpose of the Research Project】

π-Electronic molecules, displaying electronic, optical, and magnetic functions, have played critical roles not only in fundamental chemistry but also in diverse research areas from materials to life sciences. A recent innovation of organic electronics stems from the studies on π-electronic materials, originating from the discovery of organic semiconductors in 1954 by Akamatsu, Inokuchi, and Matsunaga. After years of research, including the finding of conducting polyacetylene by Shirakawa, the first organic device was developed in the 1980s. Now, the time has come for the science of π-electron systems to advance to the next stage.

Functional molecules that have realized historic breakthroughs are always structurally simple and beautiful. With this fact in mind, we will elaborate new π-electronic molecules and assemblies that hold "beautility". Our research area aims to create superb π-electronic materials and functions as well as discover new phenomena based on our design concept of "π-figuration".

【Content of the Research Project】

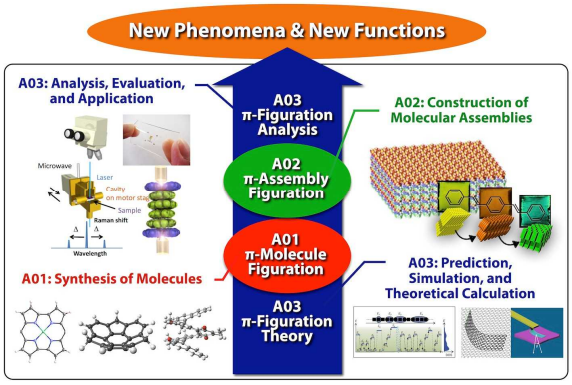
To achieve the above objectives through interactive cooperative research, we have devised the following groups:

Group A01 (π-molecule figuration) develops novel molecular frameworks that provide the basis for the π-figuration concept by utilizing state-of-the-art organic synthesis.

Group A02 (π-assembly figuration) develops functional π-electronic molecular assemblies at many length scales by utilizing state-of-the-art supramolecular and polymer chemistry.

Group A03 (π-figuration theory and analysis) predicts, designs, and unveils the functions of the new π-electronic materials by utilizing state-of-the-art theory, computational, and measurement techniques.

The dynamic motion and mechanical stimulus generated in π-electronic materials can perturb the electronic function. Harmonizing π-electronic functions with molecular dynamism should result in new phenomena and functions. As an example, we will explore the functions of π-electron systems deviated from their thermodynamically stable states by applying multiple physical stimuli (*e.g.*, an electric field, light, and magnetic field) and mechanical stimuli (*e.g.*, pressure and shear) to π-electronic molecules and their assemblies.



【Expected Research Achievements and Scientific Significance】

Our research focuses on pursing fundamental science to unlock the potential of π-electron systems rather than improving a specific material property of existing organic devices. For instance, our research would realize fundamental technologies of organic electronics based on novel operating principles. A paradigm shift in the research field of π-electronic materials should be achieved by interdisciplinary research in synthetic chemistry, materials science, and theoretical chemistry.

【Key Words】

π-electronic materials, organic chemistry, physical chemistry, polymer chemistry, supramolecular chemistry, materials science, theoretical chemistry, organic device.

【Term of Project】 FY2014–2018

【Budget Allocation】 1,143,000 Thousand Yen

【Homepage Address and Other Contact Information】

http://pi-figuration.jp