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

Broad Section E

Title of Project： **Science of Post-nanocarbons: Structural science of nano π-space**

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Research Project Number: 20H05672 Researcher Number：30302805
Keyword：Nanocarbons, Organic synthesis, Physical organic chemistry, Giant molecules, Curved-π conjugation

【Purpose and Background of the Research】

The science of nanocarbons started by the discovery of fullerenes (1985), carbon nanotubes (1991) and graphenes (2004). Currently, giant nanocarbons such as nanotubes and graphene attract much interest in particular, but there exists one big problem. These nanocarbons are a mixture of various structures and are chemical species, which hampers in-depth understanding as a molecular entity.

This study aims to design and synthesize new "nanocarbon molecules" having discrete molecular structures, which should allow for extensive explorations of their properties/functions. In this project, we wish to answer a fundamental question such as "What is the anomalous property of curved π-systems?" by designing and creating new molecules. We also aim to expand the scope of nanocarbon molecules to be applicable to other fields such as physics and materials science.

【Research Methods】

In this project, three representative topics will be explored for the development of the science of molecular nanocarbons.

(1) Creation of diverse nanocarbon structures. We will explore the scope of concise synthesis of molecular nanocarbons, which should be developed on our ground works of nanocarbon molecules (Figure 1). For example, we have started a new design strategy named "Geodesic Phenine Framework (GPF)", which utilizes a building unit of "phenine = 1,3,5-trisubstituted benzene". This method creates a series of a new class of nanocarbons, and simple chemical compositions of hydrocarbons should be the main targets of this project.

(2) Elucidation of basic characteristics. We will elucidate the basic properties of nanocarbon molecules through physical organic studies. We will employ the state-of-the-art analytical methods in combination with the theoretical and computational chemistry. By applying analytical methods to novel molecules, the characteristics of new nanocarbon molecules will be disclosed.

(3) Development of functions. We develop the unique properties of curved π-systems to functions to be applicable to materials. For instance, we have recently discovered solid-state inertial rotations of the C_{60} guest in our tubular nanocarbon host with rotational frequencies reaching over 200 GHz. The development of a functional molecular machine using such unique dynamics is one of the important subjects to be explored.

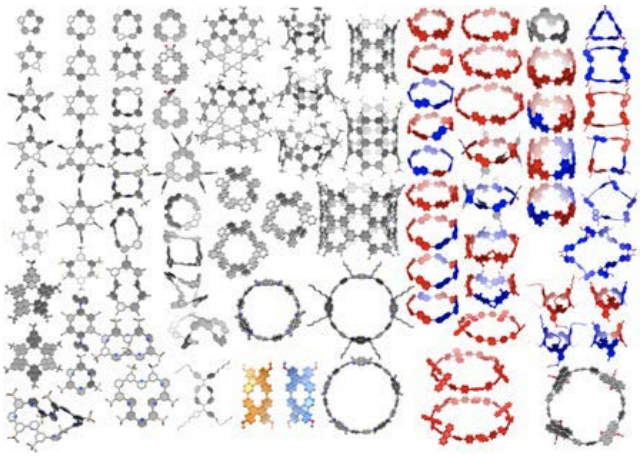

Figure 1. Representative examples of our nanocarbon molecules.

【Expected Research Achievements and Scientific Significance】

We expect the discovery of new properties of gigantic nanocarbons and, which should deepen our understanding of molecular nanocarbons. Atomic precisions that will be brought about by the present project will provide sicentific insight to gigantic and curved π-systems. Anomalous characteristics and functions of nanocarbon molecules should be explored in interdisciplinary fields, which is based on fundamental physical organic studies for (1) creation of diverse structures, (2) elucidation of basic characteristics and (3) development of functions. Design and synthesis of new functional materials shall be expected.

【Publications Relevant to the Project】

· "Ratchet-free solid-state inertial rotation of a guest ball in a tight tubualr host" Matsuno, T.; Nakai, Y.; Sato, S.; Maniwa, Y.; Isobe, H. *Nat. Commun.* **2018,** *9*, 1907.
· "Finite phenine nanotubes with periodic vacancy defects" Sun, Z.; Ikemoto, K.; Fukunaga, T. M.; Koretsune, T.; Arita, R.; Sato, S.; Isobe, H. *Science* **2019**, *363*, 151-155.

【Term of Project】 FY2020-2024

【Budget Allocation】 149,800 Thousand Yen

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