【Grant-in-Aid for Specially Promoted Research】

Science and Engineering

Title of Project： Creation of unexplored molecular nanocarbons

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【Purpose and Background of the Research】

Nanocarbons, nanometer-sized carbon materials, conduct electricity, absorb and emit light, and exhibit interesting magnetic properties. In addition to well-known nanocarbons such as spherical fullerenes, cylindrical carbon nanotubes, and sheet-shaped graphenes, theoretical simulations have predicted a number of exotic three-dimensional nanocarbon structures that have yet to be synthesized. At present, however, synthetic routes to nanocarbons almost invariably lead to mixtures of compounds displaying a range of different structures and properties; these mixtures cannot be easily separated into pure forms. The "*mixture problem*" that arises during the synthesis of nanocarbons represents one of the most significant challenges in the science and technology of nanocarbons.

The objectives of this project are (1) to design and synthesize novel nanocarbons as single structures, individually distinguishable and identifiable, and (2) to create highly advanced functional materials based on these single-molecule materials. We combine chemical and physical methods for the controlled synthesis of single-molecule nanocarbons, and conduct interdisciplinary research that encompasses the control of molecular arrangement and orientation, structural and functional analysis, and applications in devices and biology. Through this project bringing molecular science and materials science together, we aim to establish the new field of *molecular nanocarbon science*.

【Research Methods】

1. Carbon nanotubes

Carbon nanobelt is the molecule that represents the fully fused cylindrical aromatic hydrocarbon (e.g. *Science* 2017). In this project, we establish the synthetic methods of carbon nanobelts having various lengths, diameters, and structures. As a further challenge, we perform the CNT growth using carbon nanobelt as a seed to provide CNTs with uniform physical properties.

2. Graphene nanoribbons

We have synthesized graphene nanoribbons (GNRs) with various widths, edge structures, lengths, and periodic defects by using APEX reactions (e.g. *Science* 2018) developed by our group. Here we challenge to create APEX polymerization reactions to control the length of GNR precisely. Sequential oxidative annulation reaction can proceed to the formation of adjacent carbon-carbon bonds to form planar GNRs. By utilizing this technique, we synthesize various GNRs (fjord-type GNRs and armchair-type GNRs) having different width and edge structures by using precisely designed silole monomers.

3. Three-dimensional nanocarbon network

In this subject, we work on the creation of three-dimensional carbon networks that enables condensed conjugation with only carbon atoms. Three-dimensional carbon networks consisting solely of sp^2 carbon atoms are substance groups of dreams considering the theoretical prediction of outstanding physical properties. In this research, we apply molecular nanocarbon synthesis technology such as APEX reaction of aromatic compounds.

【Expected Research Achievements and Scientific Significance】

The concept of "molecularity and molecular materials" will lend new values and creativity to nanocarbon science, which is already starting to create a social ripple effect, and the creation of innovative molecular nanocarbon materials will have a huge impact on industry. Furthermore, many new methodologies and techniques for molecular synthesis and structural analysis will be developed throughout this project. Synthesis and analysis techniques are not particular to a single type of molecule or substance. Therefore, these methodologies will bring breakthroughs to many chemical, physical, or biological fields as molecular sciences.

【Publications Relevant to the Project】

・Segawa, Y.; Itami, K. *et al.*, Synthesis of a carbon nanobelt, *Science* **2017**, *356*, 172–175.

・Murakami, K.; Itami, K. *et al.*, Synthesis of partially and fully fused polyaromatics by annulative chlorophenylene dimerization, *Science* **2018**, *359*, 435–439.

【Term of Project】 FY2019-2023

【Budget Allocation】 491,500 Thousand Yen

【Homepage Address and Other Contact Information 】

http://synth.chem.nagoya-u.ac.jp