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

Exploration of molecular nanocarbon biology

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Purpose and Background of the Research

●Outline of the research

Molecular nanocarbons (structurally uniform nanometer-sized carbon materials) with unique optical, electronic, and magnetic properties have dominated the field of organic materials such as organic electronics. We have pioneered a new field of "molecular nanocarbon science" and have synthesized many structurally uniform and unique molecular nanocarbons that are important for both basic and applied research (Figure 1). Their applications in the field of organic electronics are in progress actively.

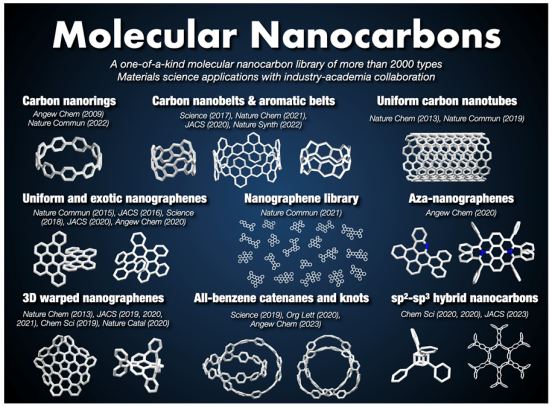

Figure 1. Our background (molecular nanocarbon synthesis and material applications)

However, due to the common sense of "carbon=material", there has been little development in the life science and drug discovery fields, with the exception of imaging. This is because molecular nanocarbons are a group of molecules that are far outside of the fixed concepts and indicators of "drug-like properties" as typified by Lipinski's law. We aim to overturn this common sense, explore the biological functions of molecular nanocarbons, and establish a new science field of molecular nanocarbon biology (Figure 2).

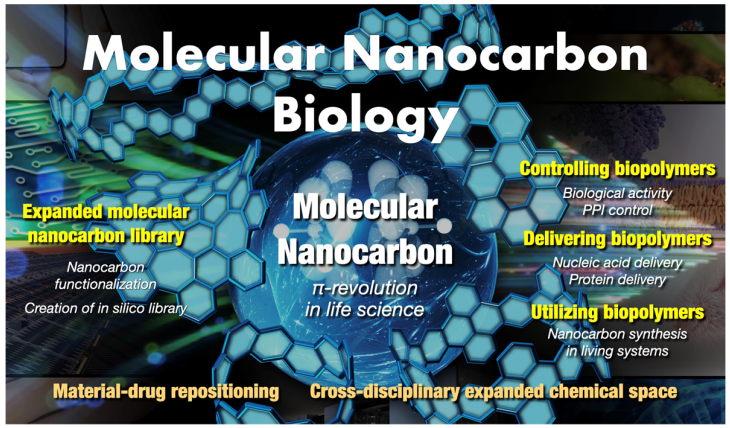

Figure 2. Overview of this project

●Purpose of this project

The purpose of this project is to create molecular nanocarbons that will revolutionize life science through molecular design and screening by actively utilizing the attractive features of molecular nanocarbons that do not exist in conventional biofunctional molecules (wide two-dimensional π-plane, flexible construction of two-dimensional and three-dimensional structures, and photo- and electron-responsive properties). Based on the world's most advanced molecular nanocarbon synthesis technology and the one-of-a-kind library of novel nanocarbon structures that have been created, as well as an in silico library that makes full use of advanced computational chemistry, we will develop molecular nanocarbons that control and transport biomacromolecules. We will also establish a completely new method for synthesizing nanocarbons in vivo using biopolymers.

Expected Research Achievements

●The approach in this project

Based on our original molecular nanocarbon library consisting of more than 2,000 types, we will develop new molecular nanocarbons that "control" and "transport" biological macromolecules. In addition, we will establish new molecule-editing methods by "using" biological macromolecules.

The detailed molecular mechanisms will then be elucidated from both computational science and molecular biology, leading to rational molecular design in a predictable way. To further accelerate this research, we will expand the existing molecular nanocarbon library from both synthetic chemistry and computational science (Figure 3).

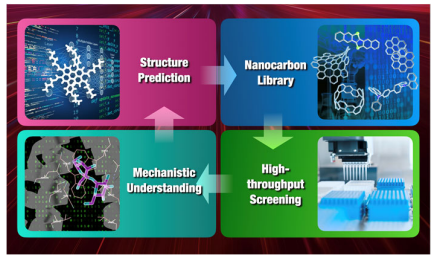

Figure 3. The approach in this project

●Expansion of molecular nanocarbon library

We will expand the molecular nanocarbon library with late-stage functionalization of the nanocarbon library that has already been constructed. We will also use advanced computational chemistry to expand the molecular nanocarbon library into the in silico domain and accelerate the bio-applications of molecular nanocarbons.

●Controlling biopolymers

We will develop new molecular nanocarbons that bind specifically to biological macromolecules. In addition, we will deeply understand their mechanisms of action from both computational science and molecular biology, and conduct large-scale bioactivity screening from both experimental and in silico approaches.

●Delivering biopolymers

Proteins and nucleic acids are being actively applied not only for basic research but also for pharmaceuticals (antibody drugs, nucleic acid drugs, etc.) and genome editing. We will develop molecular nanocarbons that transport biopolymers into cells.

●Utilizing biopolymers

We will utilize biopolymers to create novel functional molecular nanocarbons in vivo. We will utilize insects, microorganisms, and artificial metalloenzymes to develop a new "biomolecular factory" that is complementary to synthetic chemistry in flasks.

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