# [Grant-in-Aid for Specially Promoted Research]

## "Symmetry-Oriented Synthesis (SOS) Strategy" for Nanocarbon Molecular Science

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## Purpose and Background of the Research

## • Outline of the Research

This study, entitled <"Symmetry-Oriented Synthesis (SOS) Strategy" for Nanocarbon Molecular Science>, is a new chemistry project based on the development of synthetic organic chemistry. Stimulated by the emergence of "nanocarbons" such as fullerenes. carbon nanotubes and graphene, research on the chemical synthesis of nanocarbons as molecular entities is currently active. The principal investigator of this project has extensively exploited this field as one of the pioneers but believes that the budding phase of the field, in which the question was "What can be made?" is ending. We believe that we should now ask the most fundamental, the most important question: "How do we strategically synthesize macromolecules with unique symmetry and large n-electron system?" This guestion should bring further scientific development to the "retrosynthetic analysis/logic of chemical synthesis" introduced by E.J. Corey. We believe that the new nanocarbon molecules produced by this versatile SOS strategy will also reveal the mysteries hidden in nanocarbons and maximize their potential.

Design Strategy "Phenine design strategy" : A spin-out project in preceding funded research



→This project

This project (concept/idea) From "taxonomy" to "Synthetic Strategy" : Symmetry-oriented synthesis ; SOS

Symmetry-oriented retrosynthesis ; SOR

Figure 1. Symmetry-oriented synthesis

### • [Subject 1: Syntheses of challenging nanocarbon molecules by the SOS strategy]

In this research, we will attempt to deepen our symmetry-oriented synthesis strategy by setting challenging targets for the synthesis of nanocarbon molecules that are even more challenging than before, and in subject 1, we have set multiple challenging target molecules to demonstrate this new concept.

 [Subject 2: Development of synthetic tactics for the SOS strategy] In subject 2, we will develop synthetic strategies with Prof. T. Niwa as a collaborator.

#### "Symmetry-oriented synthesis" • [Subject 3: Interdisciplinary H. Isobe research with nanocarbon Strategy molecules] SOS/SOR Subject 3 of this project will explore and ChemMath (M. Kotani) develop properties and functions of Single-layer OLED (KonicaMinolta) nanocarbon molecules. Profs. Y. All-solid lithium batteries (S. Orimo) Spintropics (S Mizukami) Nakajima, T. Okamoto and R. Takehara CPL [highest g value] Stoichiometry inference (supramolecular will join this subject as collaborators to explore and develop functions of New reaction : T. Niwa Y. Nakajima : Silicon Materials nanocarbon molecules. T. Okamoto : Devices R. Takehara : Thermal Science

Figure 2. Three subjects

## Expected Research Achievements

JSPS defines the Specially Promoted Project as "an outstanding and distinctive research plan that opens up new scientific fields" and asks for a "once-in-a-lifetime challenge" of PIs. This project was made based on a panoptic view of this PI over the field including his own works, and a challenging goal was set to formulate an important concept, i.e., SOS/SOR.

In an influential book of G. Polya, "How to solve it", Polya guided us to methods of problem solving, which starts: "First, you have to understand the problem." In this regard, this PI thinks that no one has understood the problem of the nanocarbon synthesis so that they have tackled each problem in a one-off, independent manner. This project will challenge an inherent problem in the synthesis of highly symmetric molecules and form a new concept, SOS/SOR strategy, that should give us a general answer to the problem. This, I believe, will be a distinctive research that opens a new scientific field.

A representative work of PI and co-PIs is described. H. Isobe introduced a design concept of "phenine" five years ago, which led him to the synthesis of a series of phenine nanocarbons (https://doi.org/10.2183/pjab.98.020). Interdisciplinary research is another feature of his works, as can be found in a publication list in his homepage. Prof. T. Niwa is a young pioneer who explores new reactions, and his recent discovery of new Lewis-acid-mediated coupling

(https://doi.org/10.1038/s41929-021-00719-6) shows that he has the potential to make major contributions to this project. Prof. Y. Nakajima is an expert in the field of silicon chemistry, and her recent work on silica hybrids

(https://doi.org/10.1002/chem.202303159) inspired us to propose an interesting subject related to silicon materials in this project. Prof. T. Okamoto has explored cutting-edge organic materials, and his expertise in devices can lead this project to explore applications of nanocarbon molecules. Niwa/Nakajima/Okamoto have just started their professor positions in 2023. Prof. R. Takehara is a unique scientist who explores unbeaten field of thermal science (https://doi.org/10.1021/iacs.3c07921), and he and PI already started preliminary investigations of this project. This unique team will work closely together to explore the chemistry of nanocarbon molecules.

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