

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

Science and Engineering (Chemistry)



Title of Project : New Organic Chemistry and Material Science of Curved π -Conjugated Molecules

Shigeru Yamago
(Kyoto University, Institute for Chemical Research, Professor)

Research Project Number : 16H06352 Researcher Number : 30222368

Research Area : Organic chemistry

Keyword : Synthetic organic chemistry, Supramolecular chemistry, Nano carbon materials

【Purpose and Background of the Research】

Cyclic π -conjugated molecules with a curved surface as exemplified in fullerenes or carbon nanotubes (CNTs) have attracted significant attention as an active component for organoelectronic and optoelectronic materials. However, the available structure of the curved π -conjugated molecules has been quite limited as the bulk synthesis relies on physical methods. Therefore, the development of a new, selective, and practical method for bottom-up organic synthesis of novel curved π -conjugated would have significant impact both for fundamental organic chemistry and material science.

In this research project, novel curved π -conjugated molecules will be designed and synthesized in order to utilize CPP derivatives for organoelectronic materials. Through the synthesis of new molecules including host-guest complexes of curved π -conjugated molecules and the analyses of physical properties, their applications to organoelectronic devices will be examined.

【Research Methods】

The followings are four representative research topics.

- (1) **Synthesis**: By using both early- and late-stage functional group introductions, new π -extended and/or functionalized cyclic π -conjugated molecules will be synthesized.
- (2) **Formation of π -layered structure**: Construction and functionalization of the hierarchically ordered structure consisted of the curved molecules will be investigated based on the host-guest interaction.
- (3) **Evaluation of physical properties**: Physical properties of the excited and charged states of the molecules will be clarified by time-resolved spectroscopy and theoretical calculation.
- (4) **Evaluation as electronic materials**: The correlation between molecular structure, aggregation structure and physical properties will be clarified by charge transport calculation, charge mobility measurement, and aggregate structure analysis.

【Expected Research Achievements and Scientific Significance】

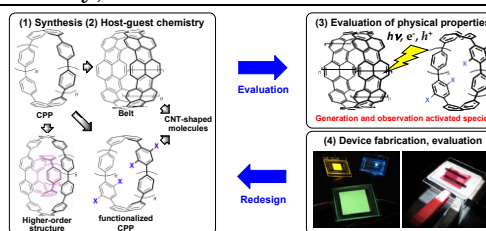


Figure 1. Main research topics

Synthesis of cyclic and curved π -conjugated molecules is a significant challenge in organic synthesis as the currently available methods are quite limited. This research will provide new curved conjugated molecules based on an innovative synthetic method and assembly by the host-guest chemistry. Furthermore, the potentials of the curved molecules for the active layer of organoelectronic devices will be clarified by the elucidation of physical properties. Through the research, a new field of organic chemistry and material science of curved π -conjugated molecules would be established.

【Publications Relevant to the Project】

- “Organoplatinum-Mediated Synthesis of Cyclic π -Conjugated Molecules: Towards a New Era of Three-Dimensional Aromatic Compounds”, S. Yamago, *et al. Chem. Rec.*, **14**, 84-100 (2014).
“Cycloparaphenylenes and carbon nanorings”, S. Yamago, *et al. Polycyclic Arenes and Heteroarenes: Synthesis, Properties, and Applications*, Qian, M. Ed., John Wiley & Sons Ltd, Chichester, UK, **2015**, pp143-162.

【Term of Project】 FY2016-2020

【Budget Allocation】 145,600 Thousand Yen

【Homepage Address and Other Contact Information】

<http://os.kuicr.kyoto-u.ac.jp/>
yamago@scl.kyoto-u.ac.jp