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

Broad Section E

Title of Project : Chemistry of Boron-Containing π-Electron Materials

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Research Project Number : 18H05261 Researcher Number : 60260618
Keyword : boron, p-electron system, planarization, supramolecular polymer, radical

【Purpose and Background of the Research】

Introduction of boron atoms into π-conjugated skeleton produces π-electron materials with characteristic electronic structures. In particular, group 13 boron can impart electron-accepting character to a π-skeleton due to an empty p-orbital of boron. For instance, triphenylborane is isoelectronic with triphenylmethyl cation and doping of boron atoms into graphene imparts semiconducting properties. In general, however, boron-containing materials are unstable due to high Lewis acidity. Steric protection of the boron center is necessary for gaining sufficient stability.

With regard to this issue, we recently found that structural constraint in a planar fashion enables producing stable boron-containing π-electron systems despite the absence of steric protection. Based on this design principle, we have so far synthesized a series of planarized boron-containing π-electron materials and investigate their characteristic properties. This chemistry can be regarded as a model study of boron-doped graphenes. Beyond this perspective, herein we aim at producing unusual properties and functions by making best use of characteristic features of planarized boron π-skeleton (Fig. 1).

【Research Methods】

Planarization of triarylboranes gives rise to 1) electron-accepting properties through effective orbital interaction between the empty p-orbital of boron and π-skeleton, 2) high Lewis acidity due to the absence of steric congestion, and 3) π-stacking ability due to the planar structure. Exploiting these features, we will pursue unusual photophysical and electronic properties and achieve controlling the self-assembled structure through the formation of supramolecular polymers. For instance, we recently developed a boron-stabilized π-radicals, which showed ambipolar carrier transporting ability in single crystal FET. We will tackle on more unusual and superb radical materials based on this type of π-skeletons. Moreover, we will synthesize various types of attractive planar π-electron materials and supramolecular polymers.

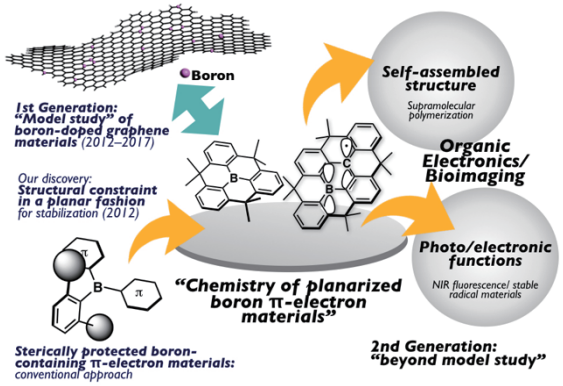

Fig. 1 Chemistry of planarized boron-containing π-electron materials

【Expected Research Achievements and Scientific Significance】

Understanding and exploitation of determinant factors of elements that govern materials functions are a fundamental issue of chemistry. Our approach in this project would contribute to progress not only in organoboron or main-group chemistry, but also in materials science, particularly organic electronics. Application to bioimaging would be also an important direction of this chemistry.

【Publications Relevant to the Project】

・T. Kushida, S. Shirai, N. Ando, T. Okamoto, H. Ishii, H. Matsui, M. Yamagishi, T. Uemura, J. Tsurumi, S. Watanabe, J. Takeya, S. Yamaguchi, *J. Am. Chem. Soc.*, **139**, 14336-14339 (2017).
・Z. Zhou, A. Wakamiya, T. Kushida, S. Yamaguchi, *J. Am. Chem. Soc.*, **134**, 4529-4532 (2012).

【Term of Project】 FY2018-2022

【Budget Allocation】 149,000 Thousand Yen

【Homepage Address and Other Contact Information】

http://orgreact.chem.nagoya-u.ac.jp/olddocs/Home.html