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

Broad Section E

Title of Project： Soft materials science based on structural two-dimensionality

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Keyword：two-dimensional molecular assembly, soft materials, organic film, self-assembled monolayer, triptycene

【Purpose and Background of the Research】

As represented by graphene, transition metal chalcogenides, and van der Waals materials, two-dimensionality is an important structural element for generating various new functions. In contrast to inorganic and carbon-based materials, no rational approach has been established for constructing a two-dimensional (2D) organic assembly while controlling the arrangement and orientation of the constituent molecules. In this study, we will establish a new design strategy for creating 2D organic materials using tripodal triptycene-based "2D supramolecular scaffolds" (Figure), which exhibit an excellent self-assembling property to form a 2D honeycomb structure through nested packing of the three benzene blades. Using this supramolecular scaffold, we will assemble various functional molecular building blocks with controlling their arrangement and orientation into a wide range of 2D material forms, including monolayers on solid surfaces, multilayer films, and even bulk crystals and polymer assemblies. We will explore emergent functions and phenomena arising from particular homo- and hetero-interfaces with designed chemical and physical properties.

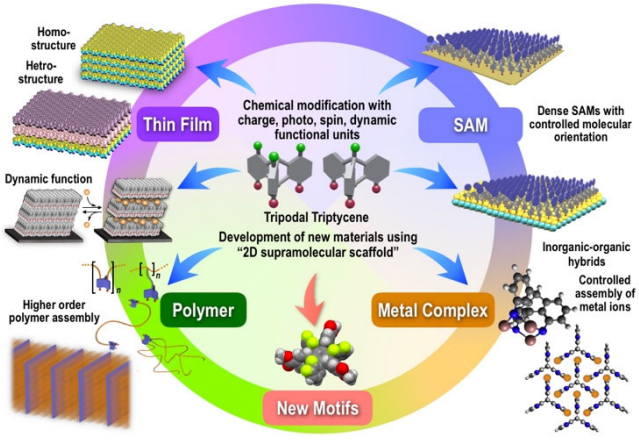

Figure. Scope of ordered 2D organic assemblies with controlled arrangement and orientation of functional molecular units, which can be constructed using tripodal triptycene as a 2D supramolecular scaffold.

【Research Methods】

We will prepare 2D molecular assemblies with diverse and unique functions by attaching small functional molecules, polymers, and metal ions to strategically designed triptycene-based scaffolds and seek for new functions of organic molecules and polymers by taking advantage of their unique properties, rather than aiming to mimic the properties and functions of inorganic and carbon-based materials. We will investigate emergent functions related to charge, spin, chirality, and mechanical properties, which arise from the interaction between functional groups incorporated with dimensionally controlled orientation and arrangement. More specifically, we will focus on the following systems: (i) 2D assembly of π-electronic units, (ii) 2D organic-inorganic hybrid materials by complexation of triptycene with main-group elements and transition metals, (iii) 2D assembly of redox active triptycenes, (iv) 2D assembly capable of cooperative collective molecular motion, aiming to develop soft actuators, (v) Higher order polymer assembly by incorporating triptycene units into polymer main-chains, pendants, and terminal groups.

Besides tripodal triptycenes, we will develop new molecular motifs capable of spontaneous 2D assembly.

【Expected Research Achievements and Scientific Significance】

The scope of materials to which our 2D assembly approach using the supramolecular scaffold can be applied is very broad, ranging from small molecules with functional units, such as π-electrons, spin, dipole, and dynamic rotor, to polymers and transition metal complexes. Along with its scientific aspects, this study is expected to lead to technological merits. For example, since 2D structures are compatible with surface, our approach would enable not only flexible design of surface structures and properties but also specific adhesion between dissimilar materials. There is no rational approach that can be generally applied to a wide variety of material systems and forms, with the keyword of two-dimensionality in organic materials. The results obtained through this research are expected to have an impact on materials science and engineering.

【Publications Relevant to the Project】

- F. Ishiwari, G. Nascimbeni, E. Sauter, H. Tago, Y. Shoji, S. Fujii, M. Kiguchi, T. Tada, M. Zharnikov, E. Zojer, T. Fukushima, *J. Am. Chem. Soc.* **2019**, *141*, 5995–6005.
- F. Ishiwari, Y. Shoji, T. Fukushima, *Chem. Sci.* **2018**, *9*, 2028–2041.
- N. Seiki, Y. Shoji, T. Kajitani, F. Ishiwari, A. Kosaka, T. Hikima, M. Takata, T. Someya, T. Fukushima, *Science* **2015**, *348*, 1122–1126.

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