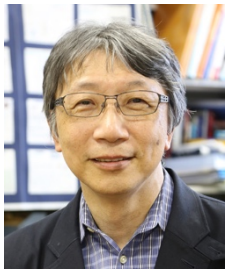
【Grant-in-Aid for Specially Promoted Research】

Science and Engineering



Title of Project： **Chemistry and Physics of Molecular Systems with Mathematically-Defined Strong Isotropic Lattice Structures**

AWAGA Kunio
(Nagoya University, Graduate School of Science, Professor)

Research Project Number: 20H05621 Researcher Number：10202772
Keyword：Strong isotropy, Geometric topology, Band-filling control

【Purpose and Background of the Research】

While the carbon materials, such as graphite, diamond, and nanocarbons, has been studied extensively, the graph theory recently has predicted the K_4 structure as a new carbon allotrope. It is mathematically demonstrated that only the three lattices, namely honeycomb, diamond and K_4, which are lattices of the carbon allotropes, exhibit the property of "strong isotropy". It is notable that the band structures of the three carbon allotropes include exotic band dispersions, which are characterized as Dirac cone, Dirac nodal line and triplet Dirac cone, respectively. Therefore, if the Fermi levels can be freely controlled in them, Dirac fermion systems would be newly constructed. However, it is hard to realize this idea in the carbon allotropes, so that we propose to make molecular mimics of the carbon allotropes, and then to carry out the band filling controls, taking advantage of their porous structures and redox activities. The purpose of this project is to exploit the electronic/spin functions originating from the topology of strong isotropic lattices, developing electrochemical band-filling control. We also elucidate the solid-state electrochemical functions, derived from the synergetic effects between electron and ion transport in the molecule-based strong isotropic lattices.

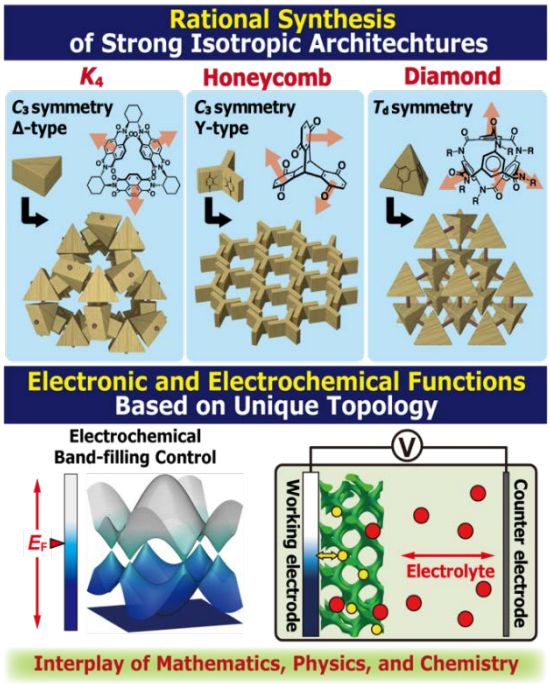


Figure 1 Research concept

【Research Methods】

1. Rational Synthesis

We work on a new methodology for making molecule-based strong isotropic materials, using "polyhedral π-conjugated molecules" with the C_3 or T_d symmetry. They respectively play the roles of sp^2 or sp^3 carbon in the carbon allotropes, to form their molecular mimics.

2. Electrochemical Band-filling Control

The band structures of molecule-based strong isotropic materials authentically include Dirac cones and flat bands. After confirming these band structures by the angle-resolved photoelectron spectroscopy and the scanning tunneling spectroscopy, we carry out the electrochemical hole/electron doping to these bands without destroying the framework lattices.

3. *Operando* Measurements

We have already developed the *operando* measurement systems on XAFS, XRD, NMR, etc. under solid-state electrochemical reactions. The present research on the strong isotropic materials is conducted under the guidance of these *operando* measurements.

【Expected Research Achievements and Scientific Significance】

Combining physics and mathematics of strong isotropy by means of chemistry, we contribute to the science and technology of topological materials. Establishing the authentic ways to form Dirac cones and flat bands, and the methodology of electrochemical band filling control, we develop novel electronic functions. The electrochemical functions such as high energy storage are also realized.

【Publications Relevant to the Project】

・ A. Mizuno, Y. Shuku, M. M. Matsushita, M. Tsuchiizu, Y. Hara, N. Wada, Y. Shimizu, and K. Awaga, "3D Spin-Liquid State in an Organic Hyperkagome Lattice of Mott Dimers", *Phys. Rev. Lett.*, **119**, 057201 (2017).
・ A. Mizuno, Y. Shuku, and K. Awaga, "Recent Developments in Molecular Spin Gyroid Research", *Bull. Chem. Soc. Jpn.*, **92**, 1068-1093 (2019).

【Term of Project】 FY2020-2024

【Budget Allocation】 426,500 Thousand Yen

【Homepage Address and Other Contact Information】

http://advmat.chem.nagoya-u.ac.jp
awaga.kunio@b.mbox.nagoya-u.ac.jp